Supporting information

Synthesis and prospective study of the use of thiophene thiosemicarbazones as signaling scaffolding for the recognition of anions

M. Manuela M. Raposo, Beatriz García-Acosta, Tatiana Ábalos, Pilar Calero, Ramón Martínez-Máñez, José Vicente Ros-Lis and Juan Soto

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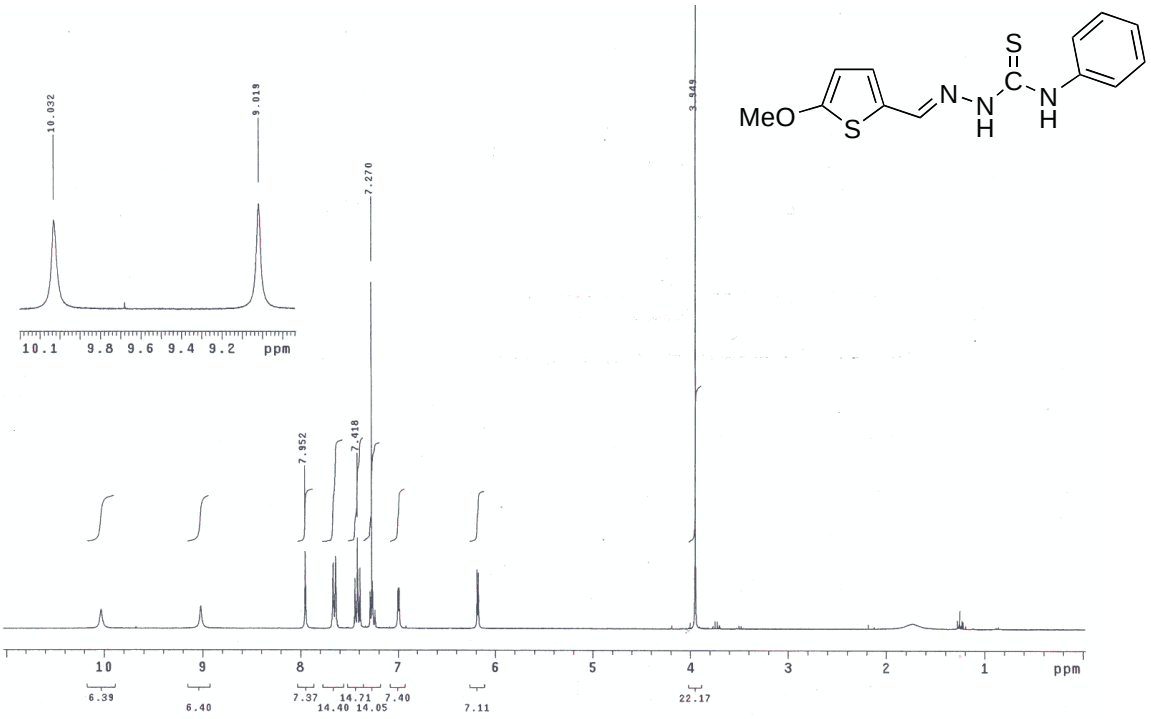
^{1}H NMR spectrum of compound **1**



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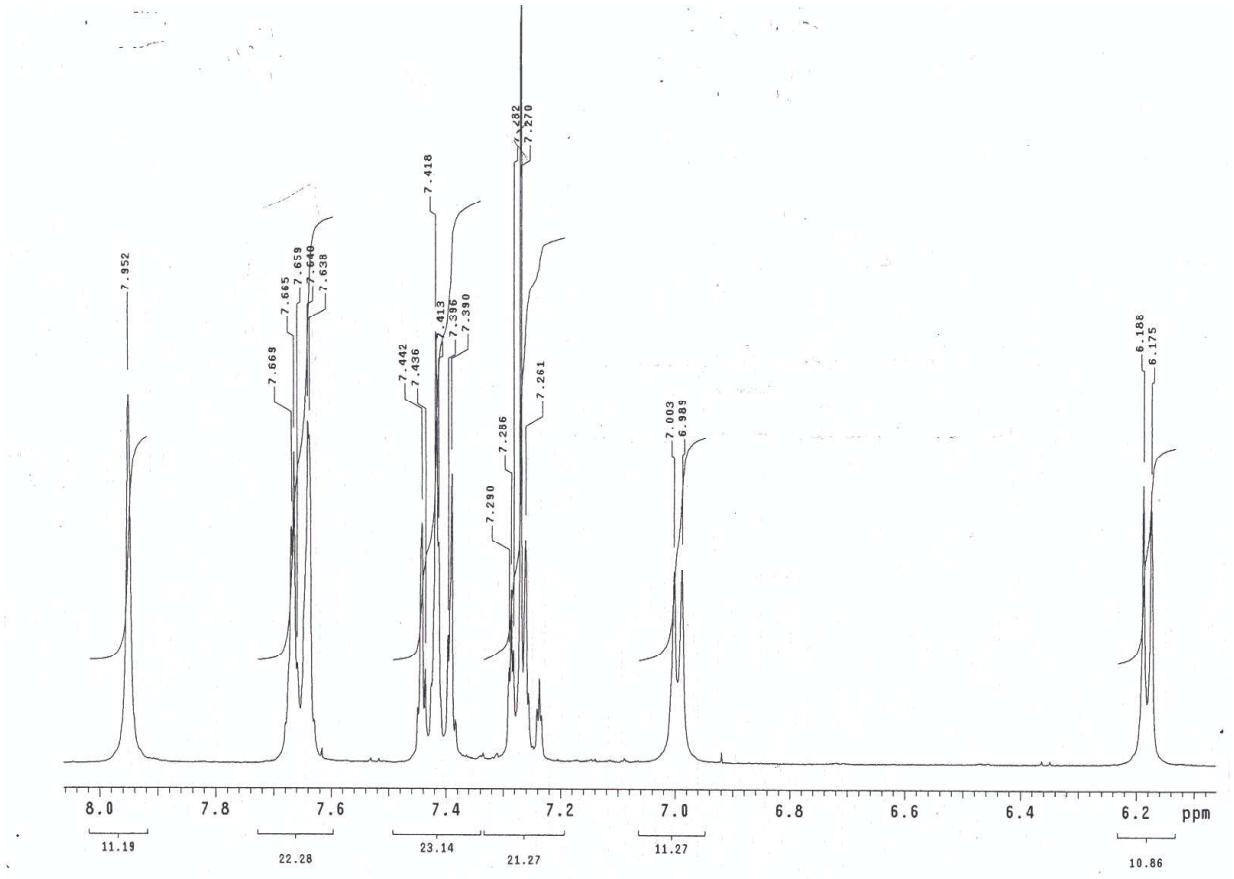
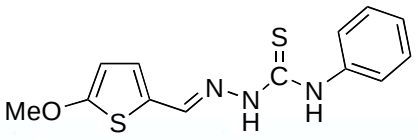


^{13}C NMR spectra of compound **1**



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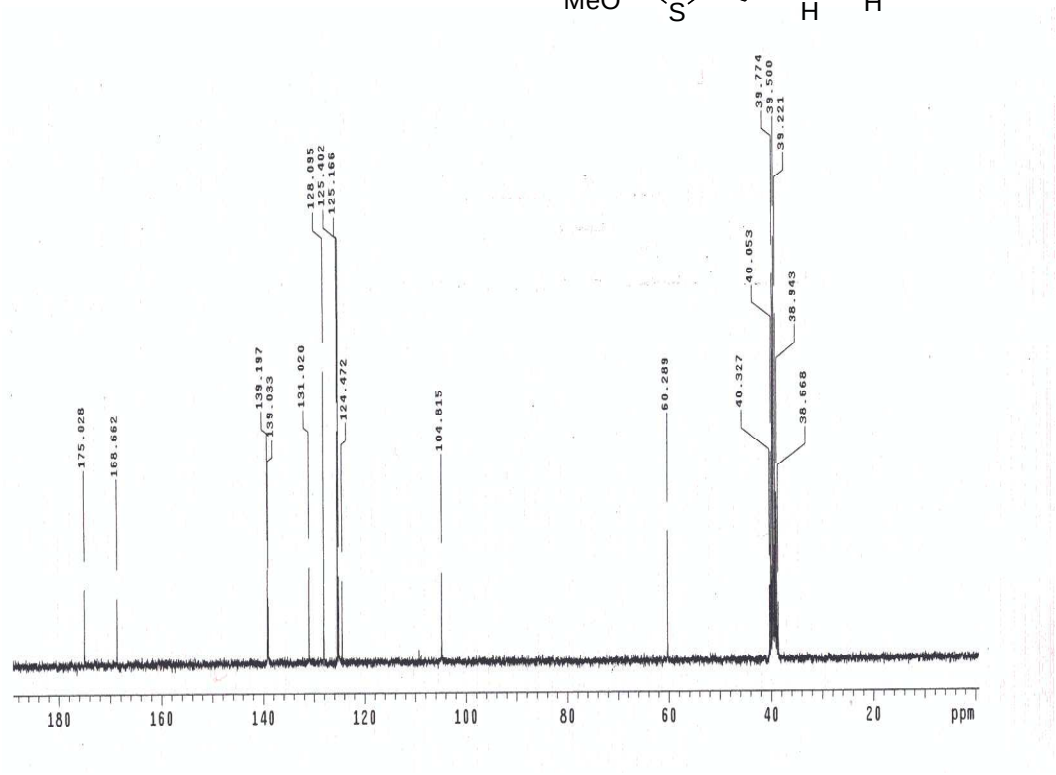
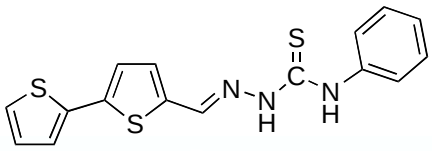


^{1}H NMR spectra of compound **2**



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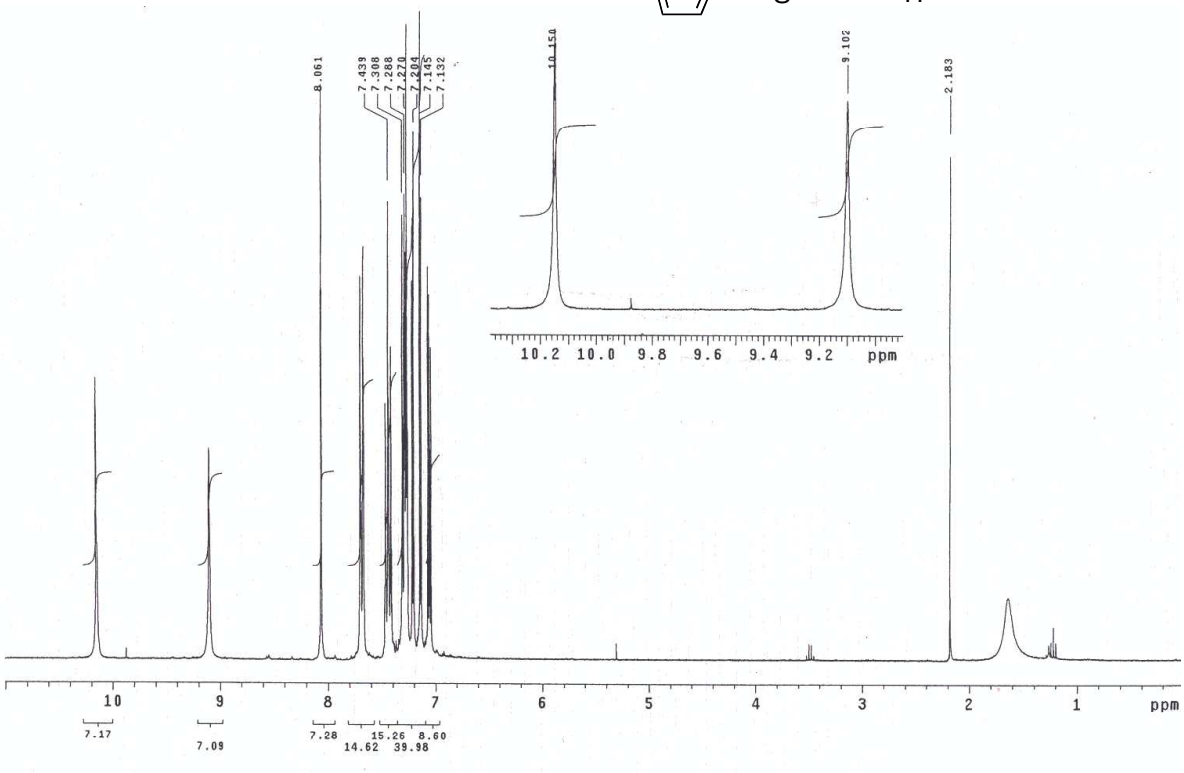
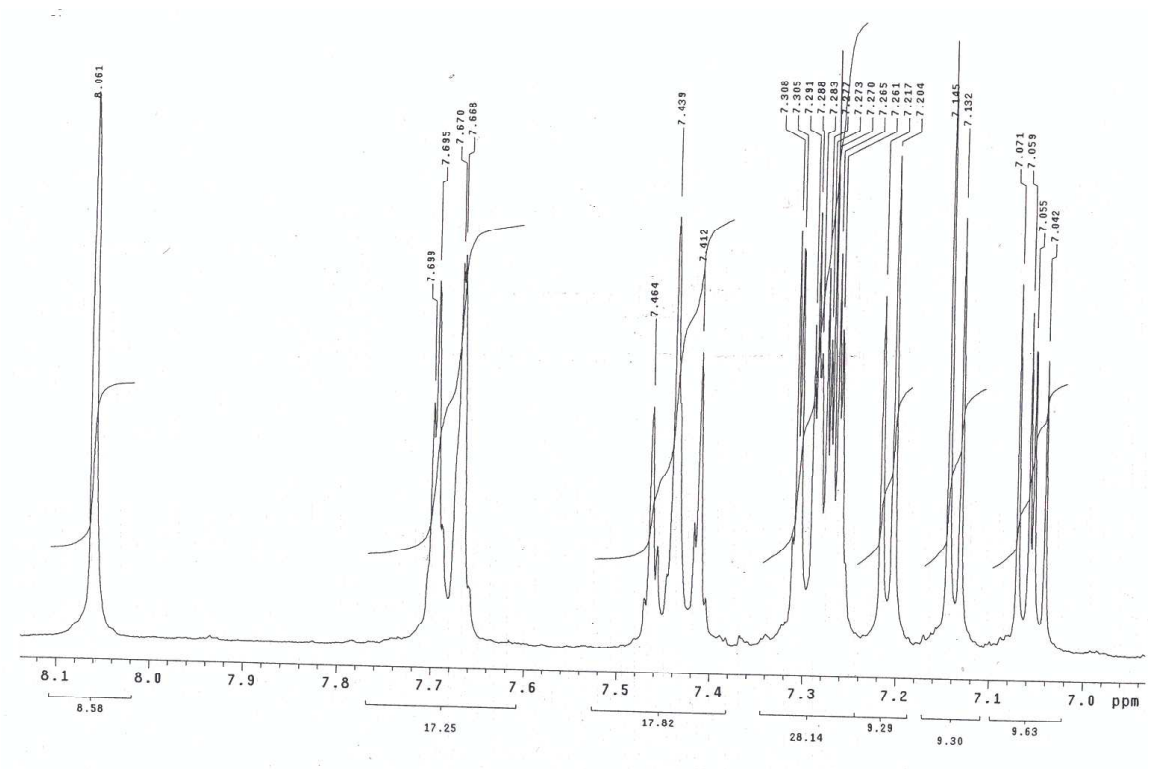
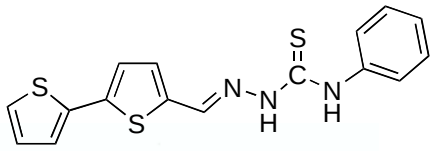




^{13}C NMR spectra of compound **2**



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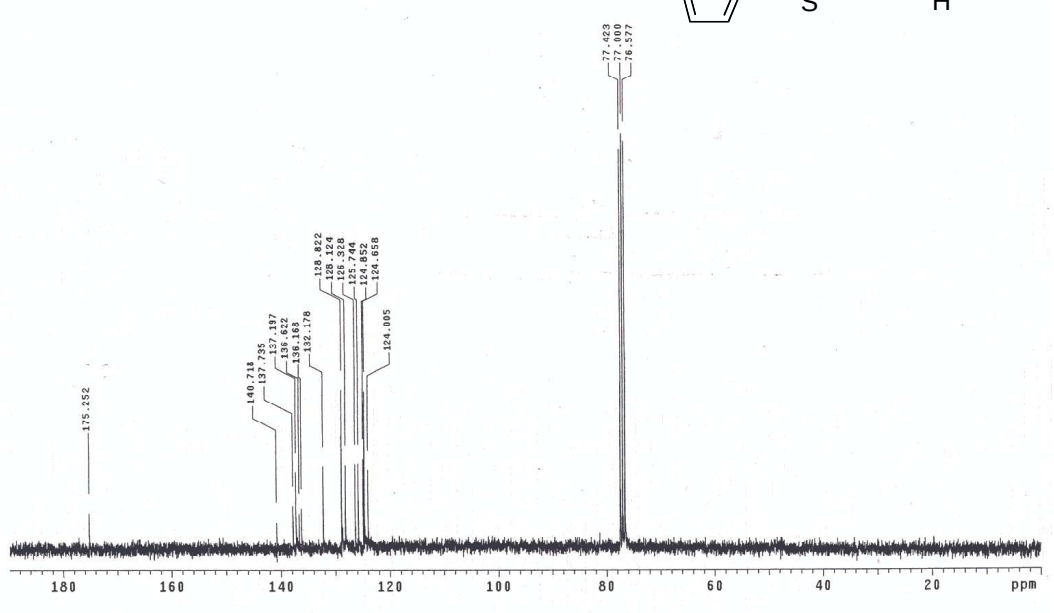

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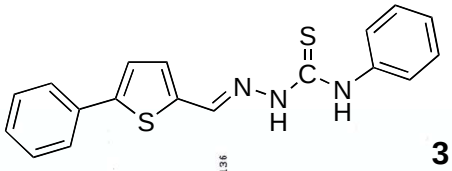

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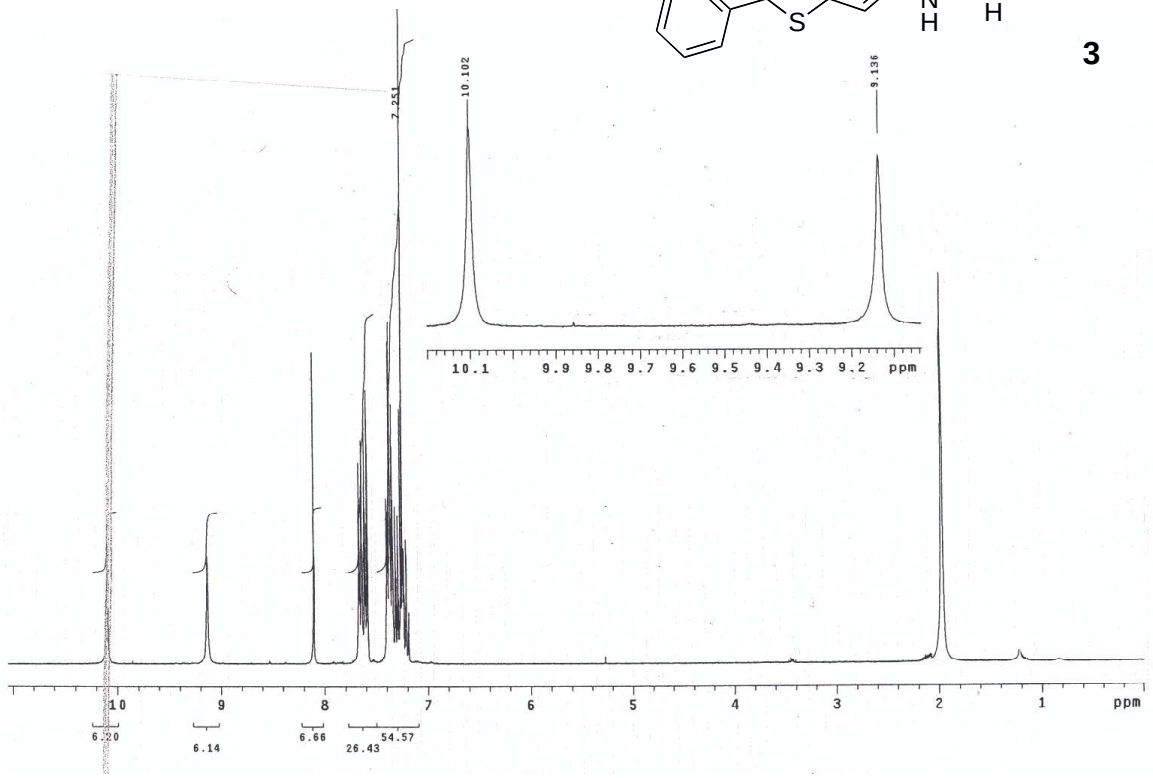

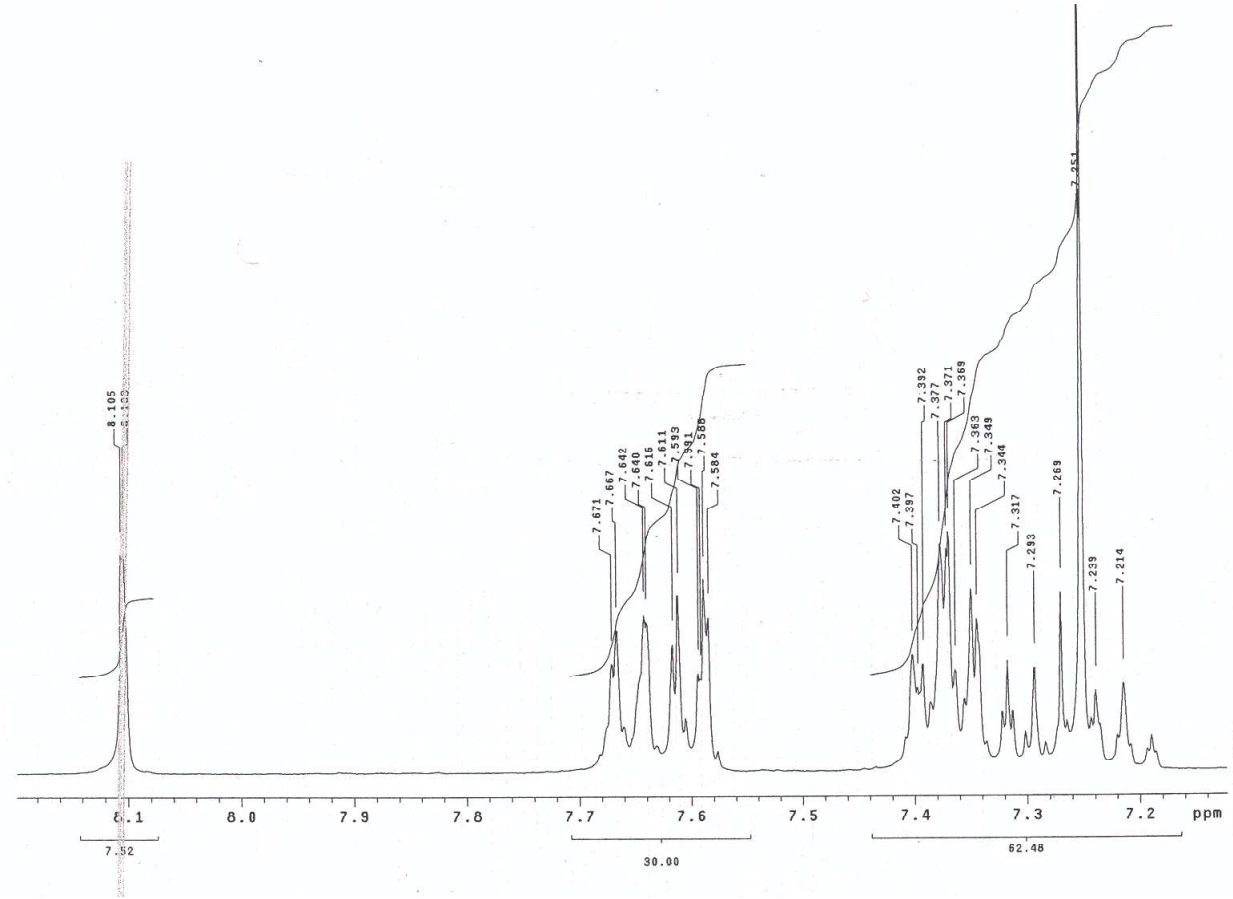

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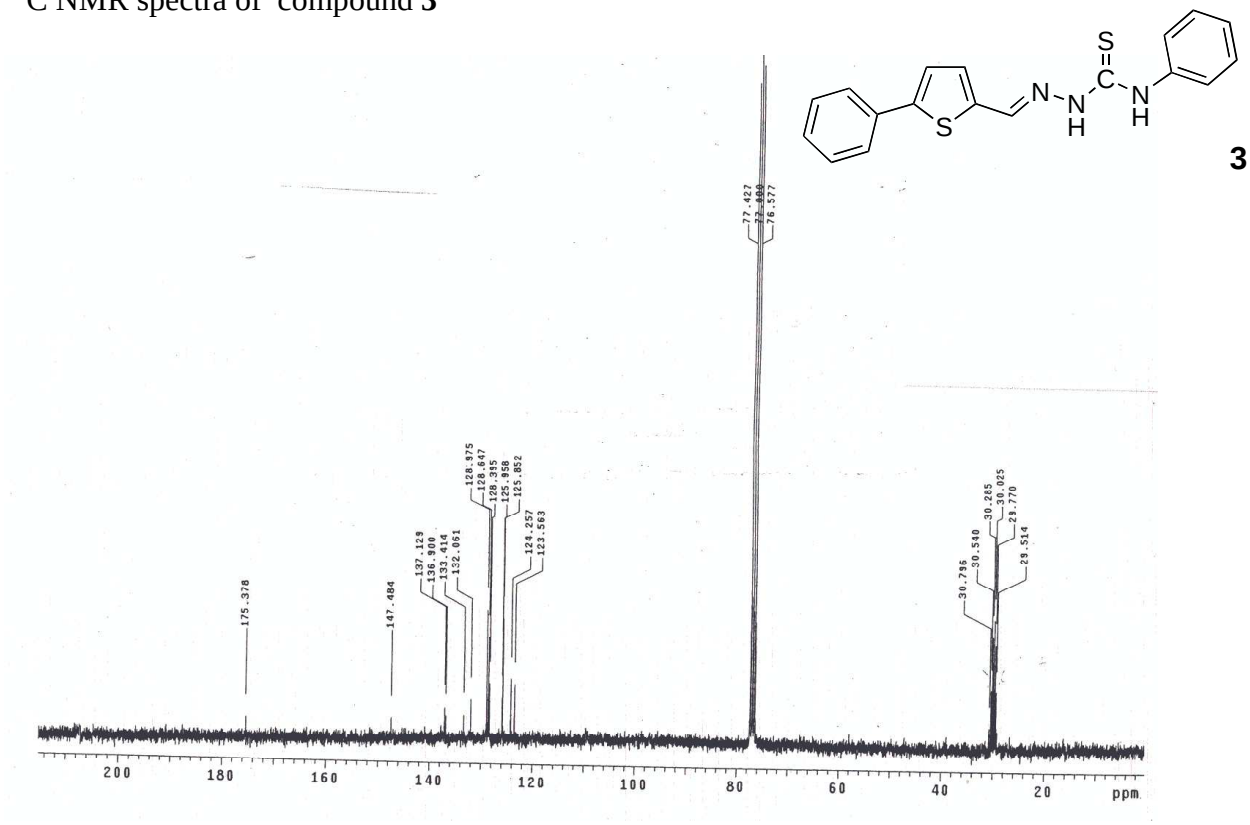
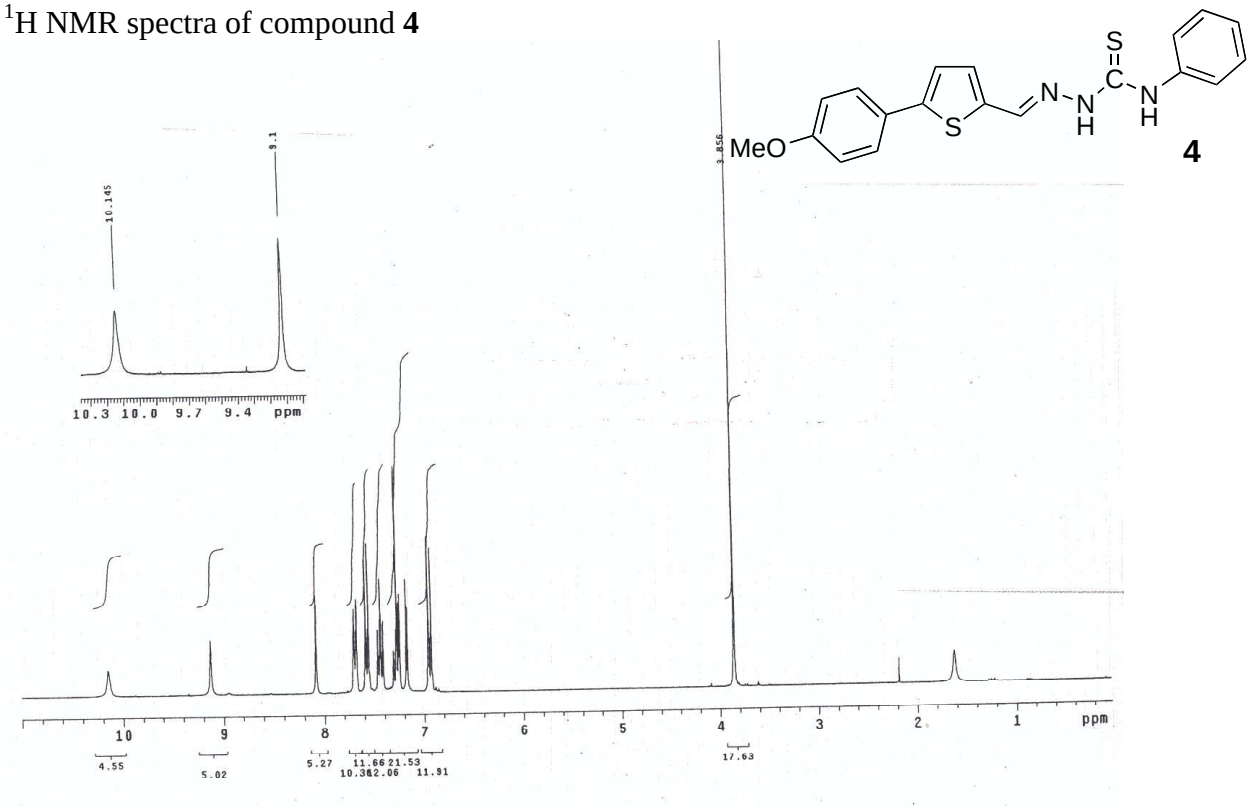
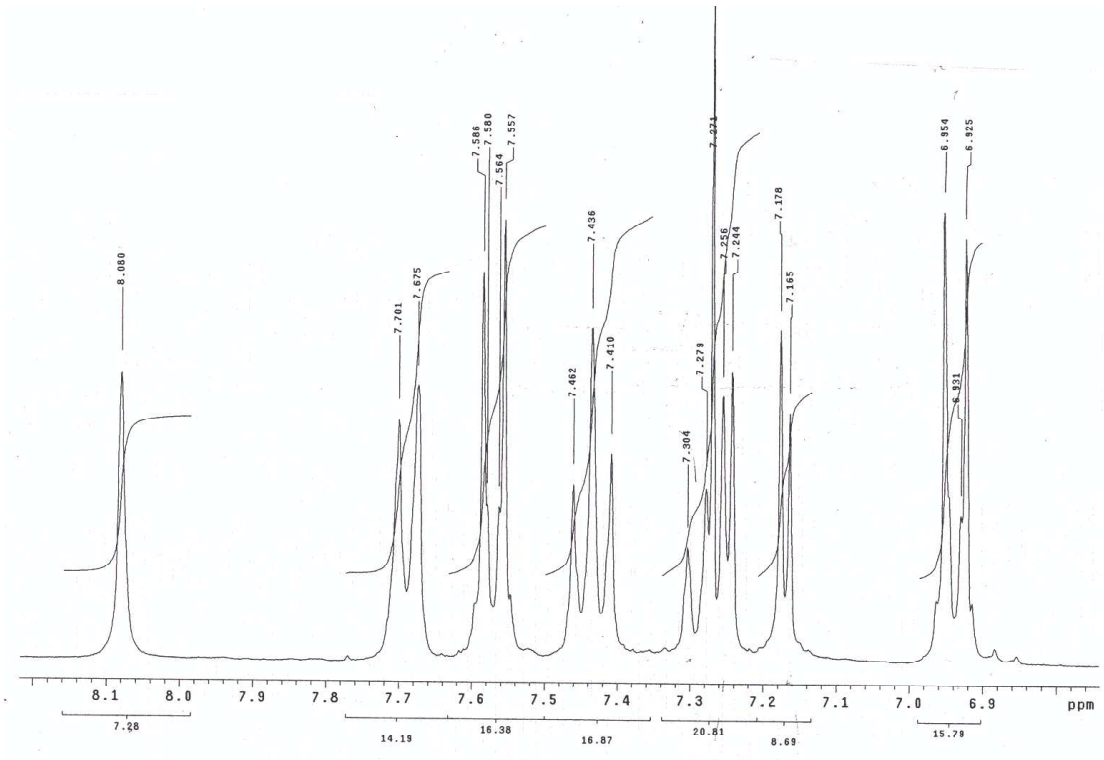
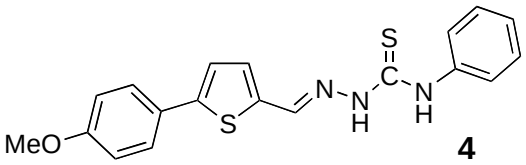


^{1}H NMR spectra of compound **4**





^{13}C NMR spectra of compound **4**



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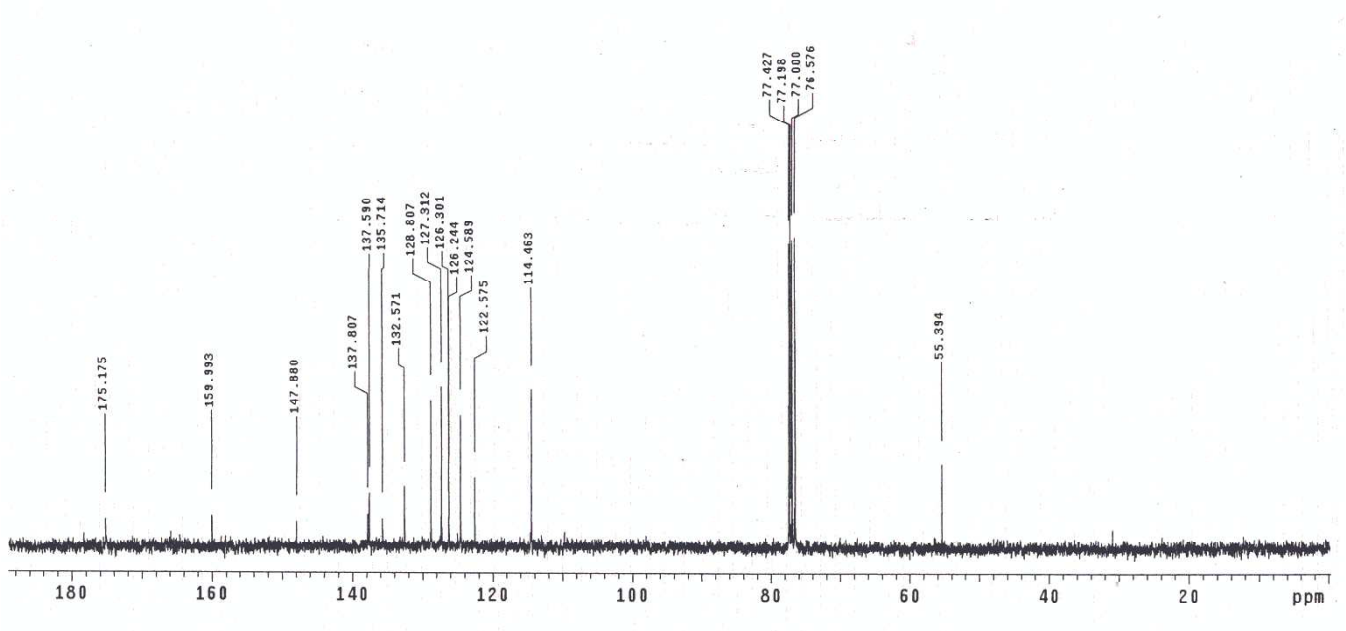

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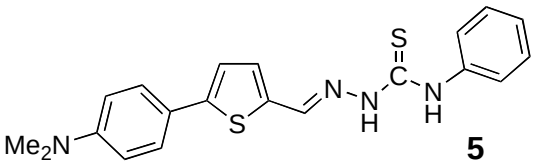

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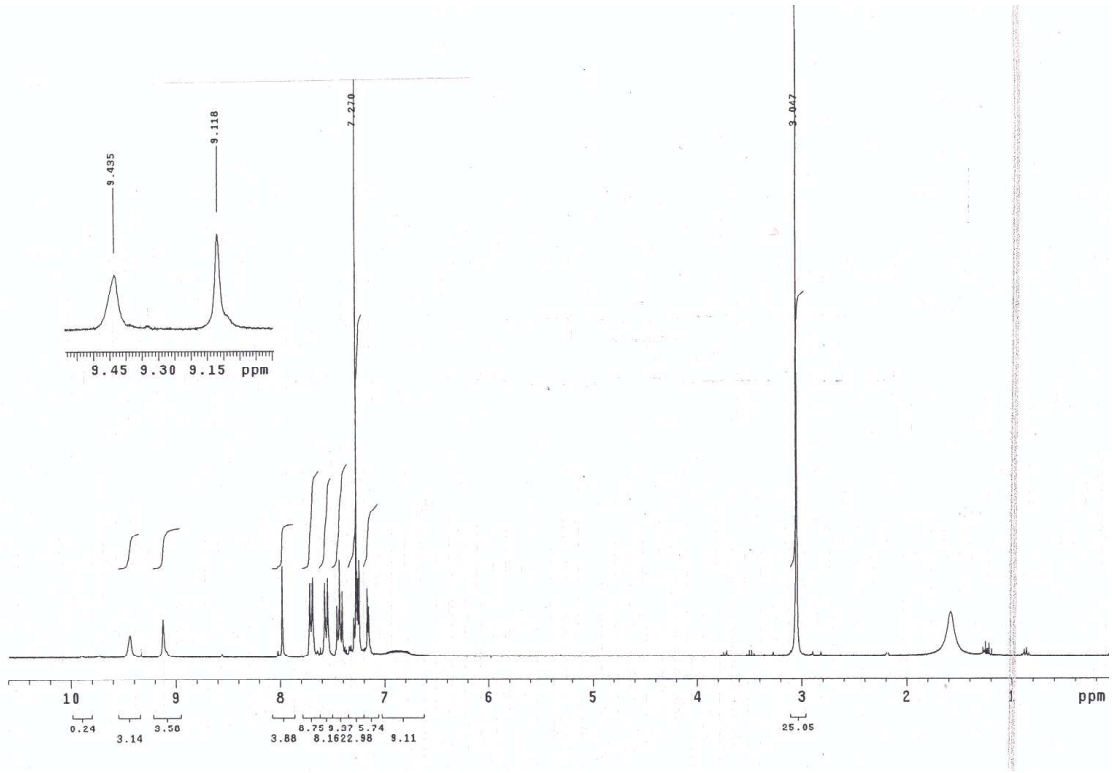

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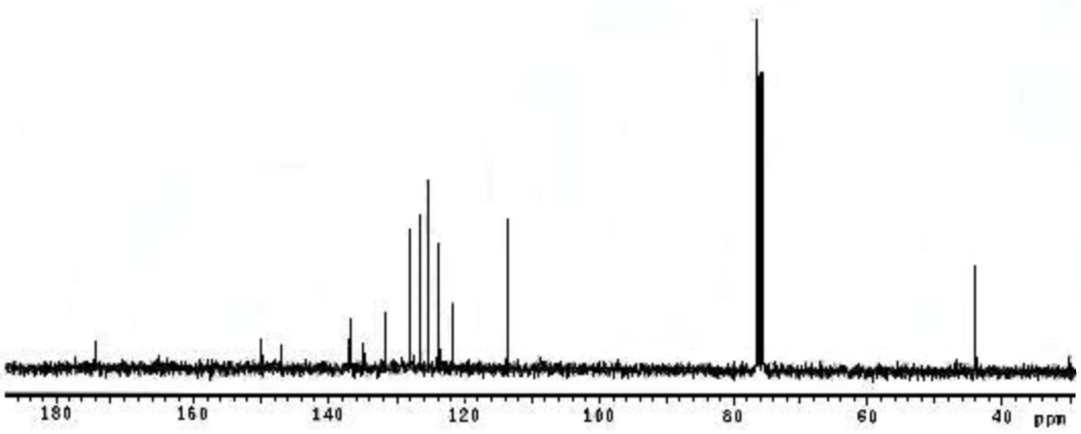

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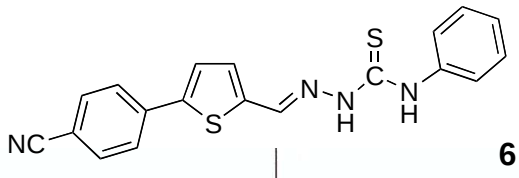

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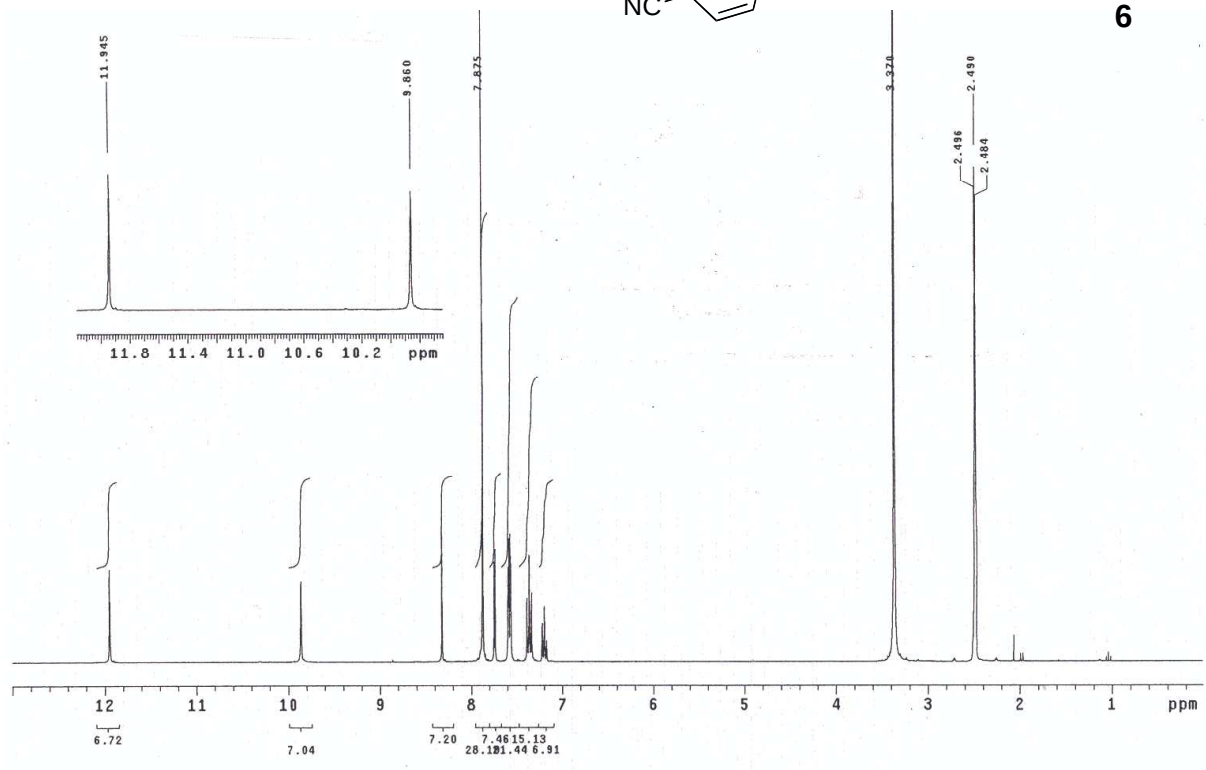

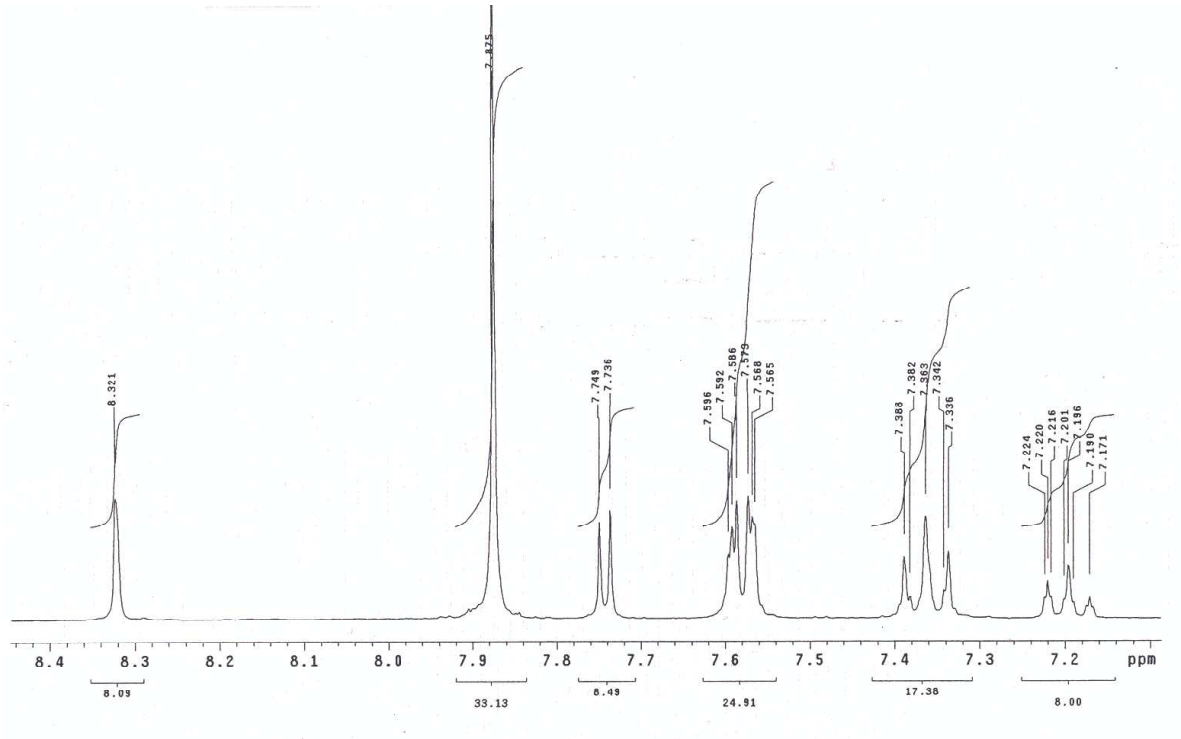

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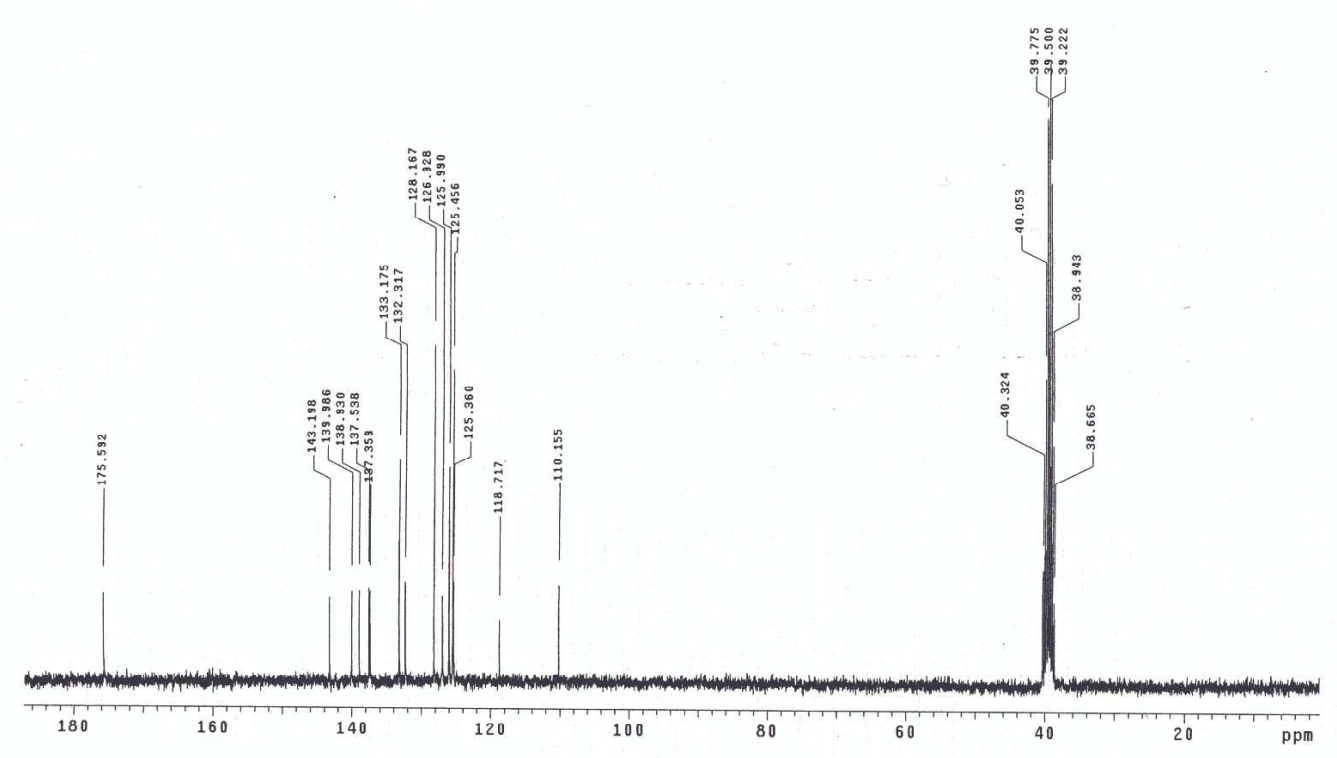
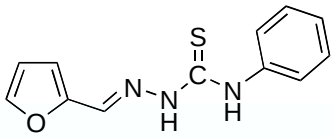


^{1}H NMR spectra of compound **7**



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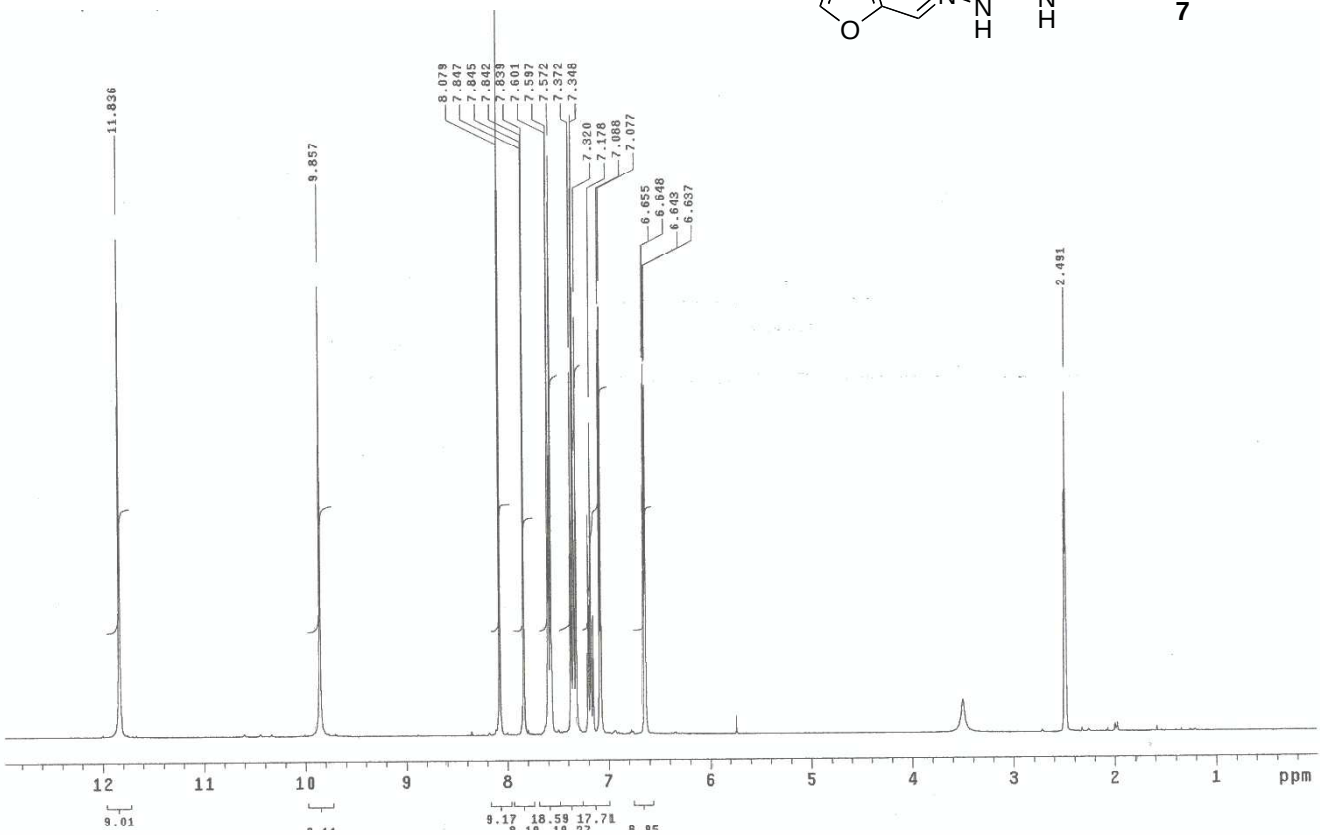
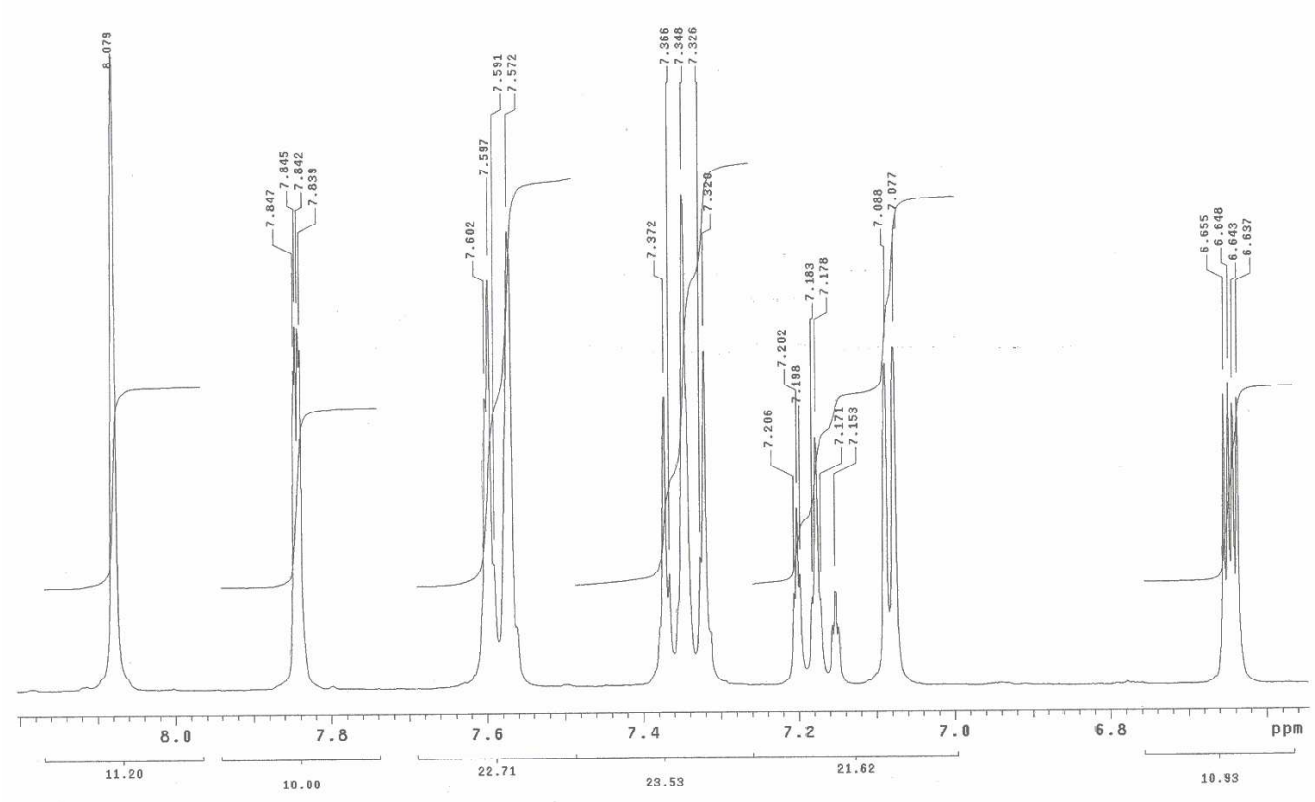
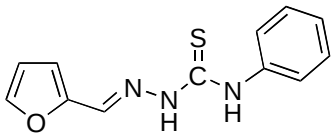




^{13}C NMR spectra of compound **7**



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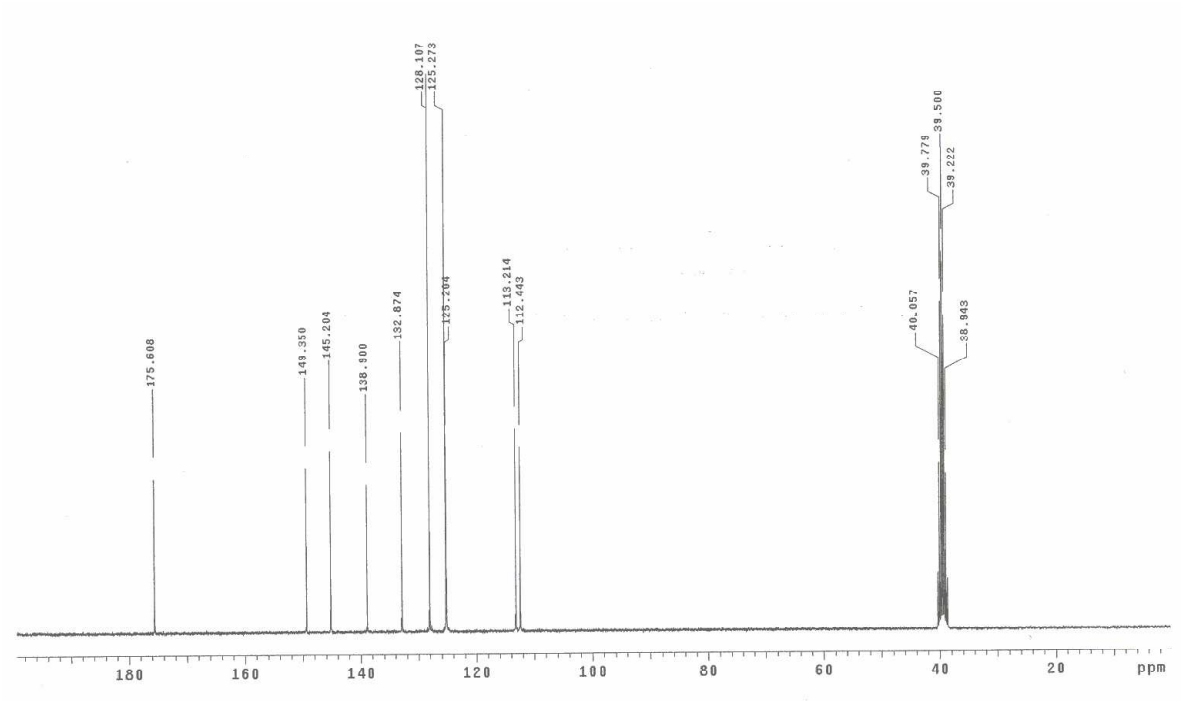
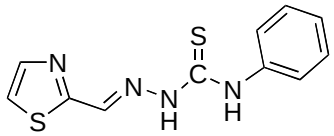


^{1}H NMR spectra of compound **8**



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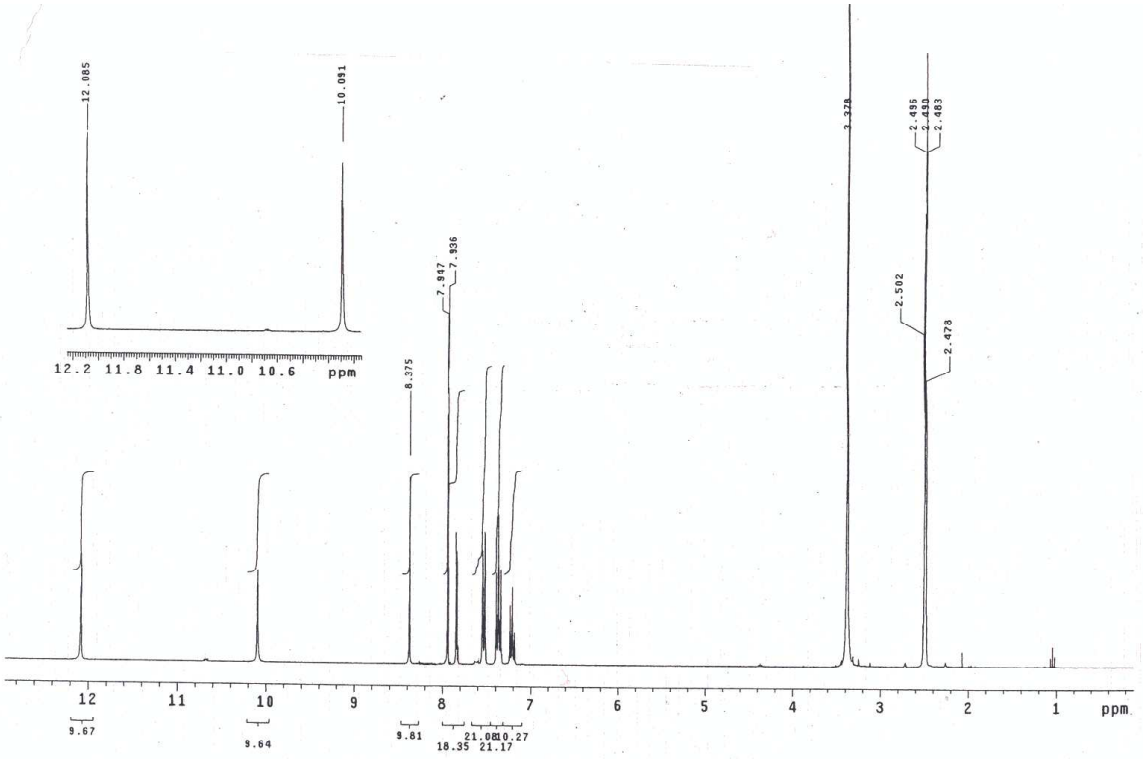

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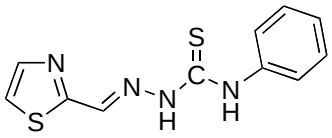

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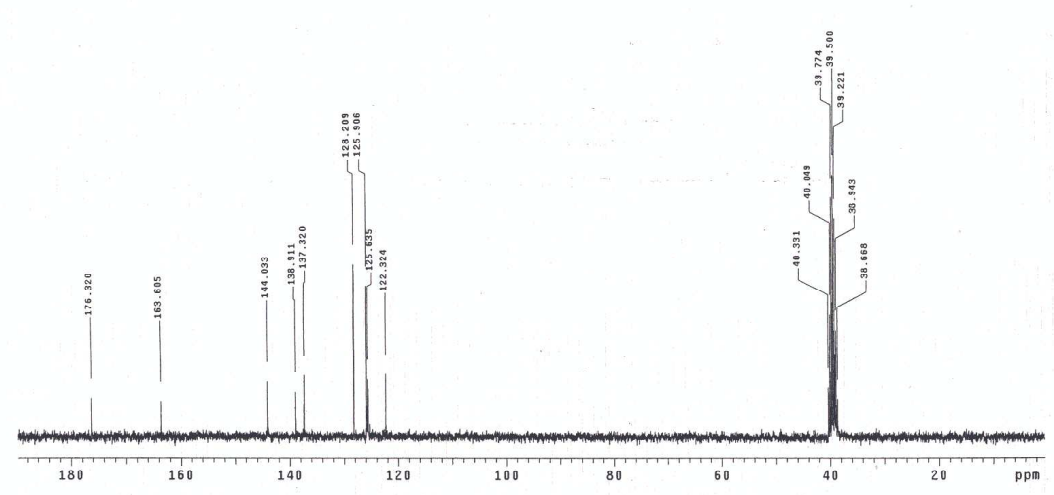
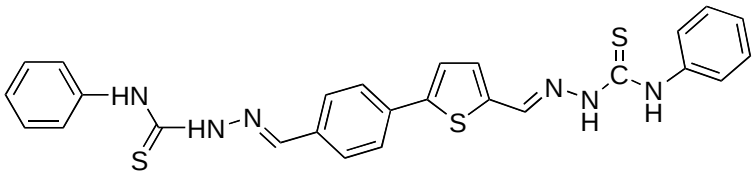


^{1}H NMR spectra of compound **9**



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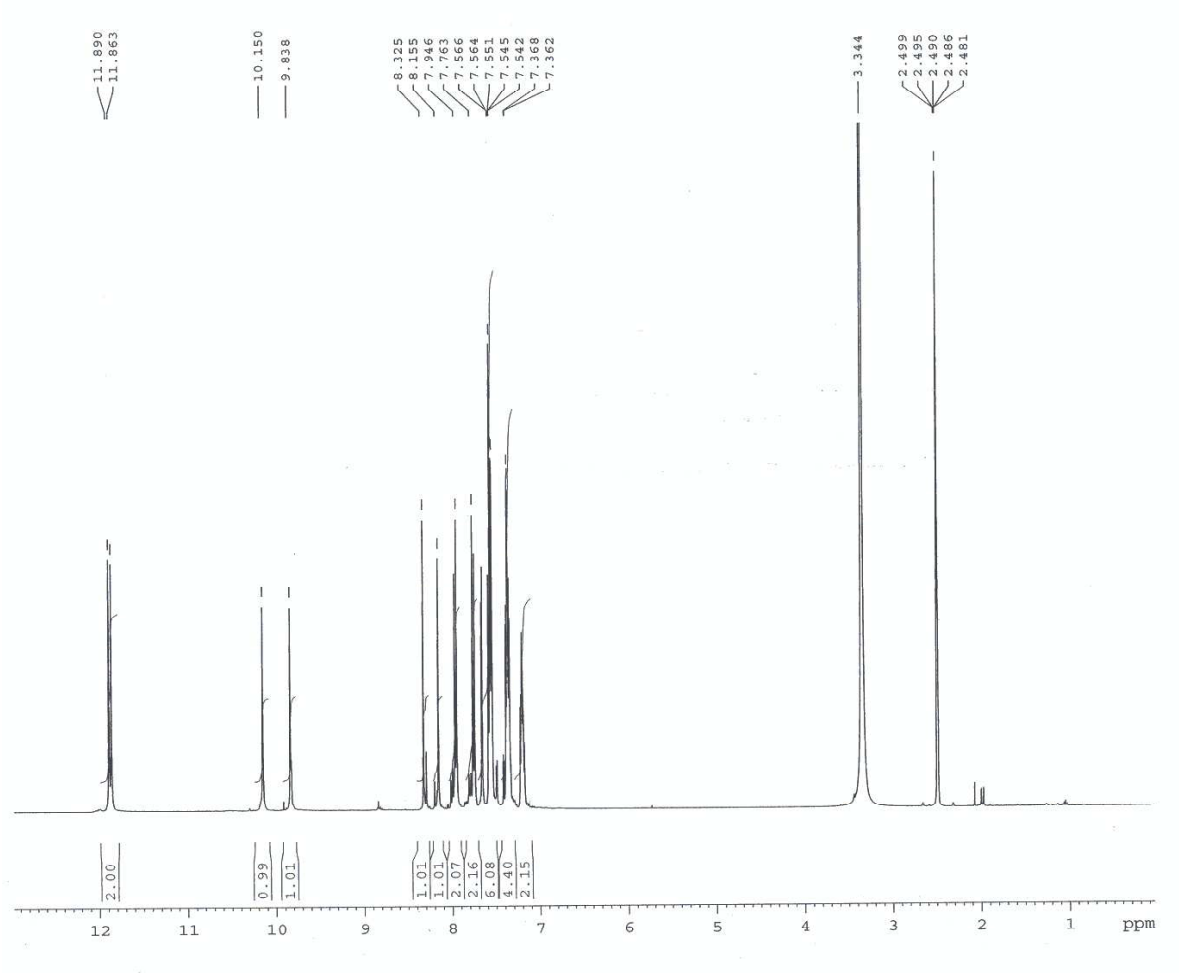

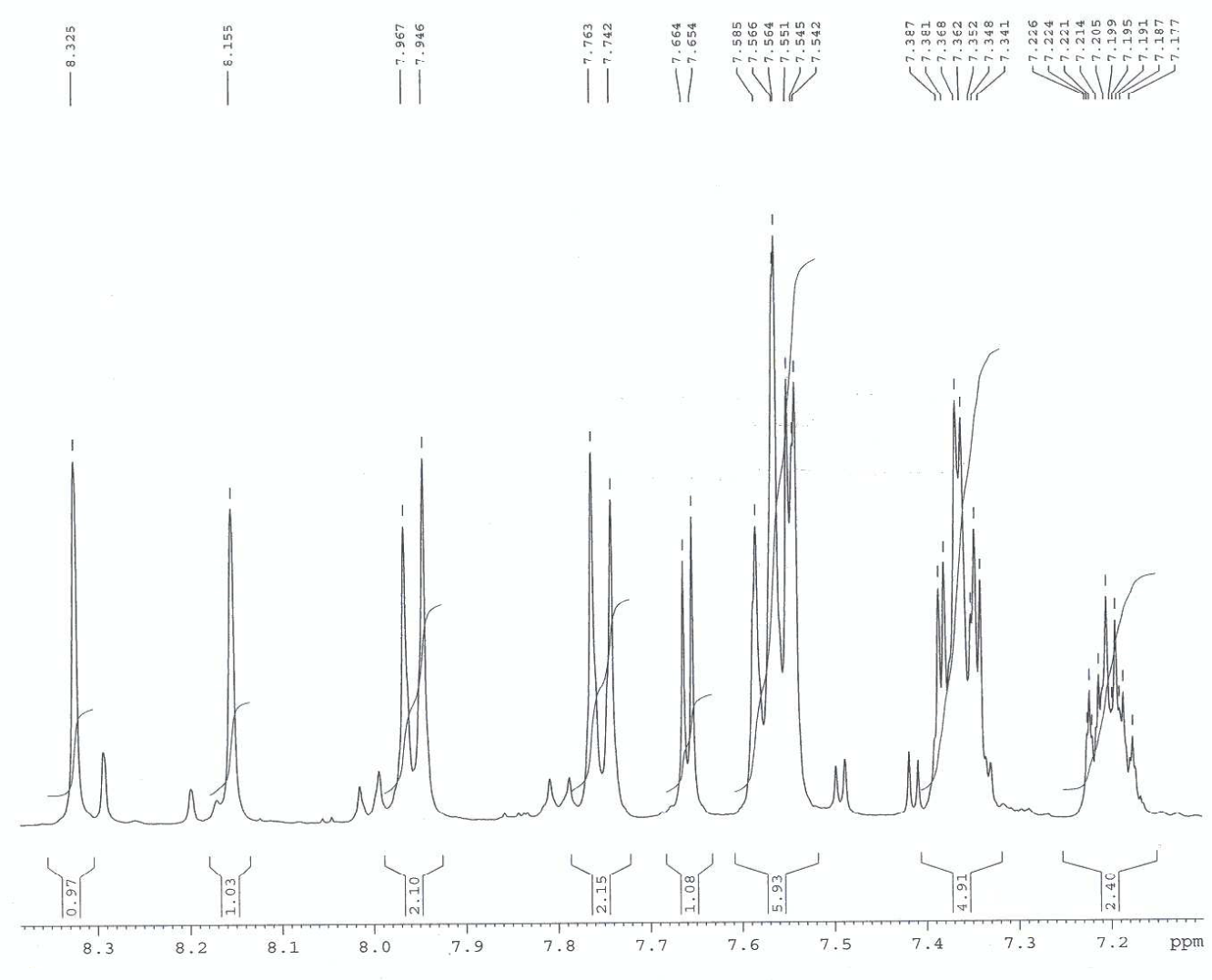
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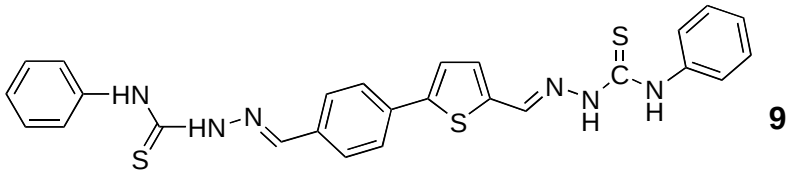
8.155
7.967
7.946
7.763
7.742
7.664
7.654
7.585
7.566
7.564
7.551
7.545
7.542
7.387
7.381
7.368
7.362
7.352
7.348
7.341
7.226
7.224
7.221
7.214
7.205
7.199
7.195
7.191
7.187
7.177
0.97
1.03
2.10
2.15
1.08
5.93
4.91
2.40
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
ppm

^{13}C NMR spectra of compound **9**



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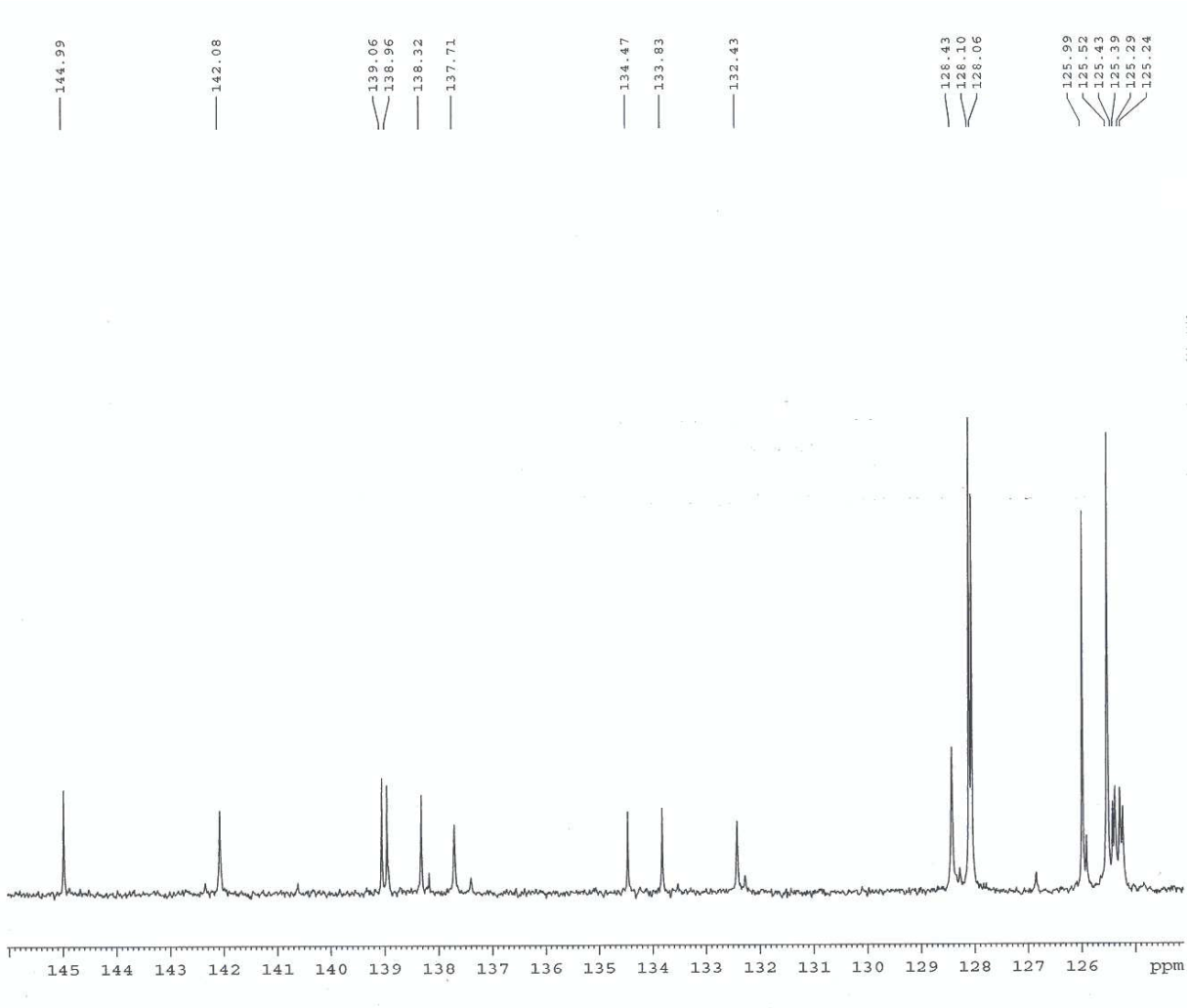

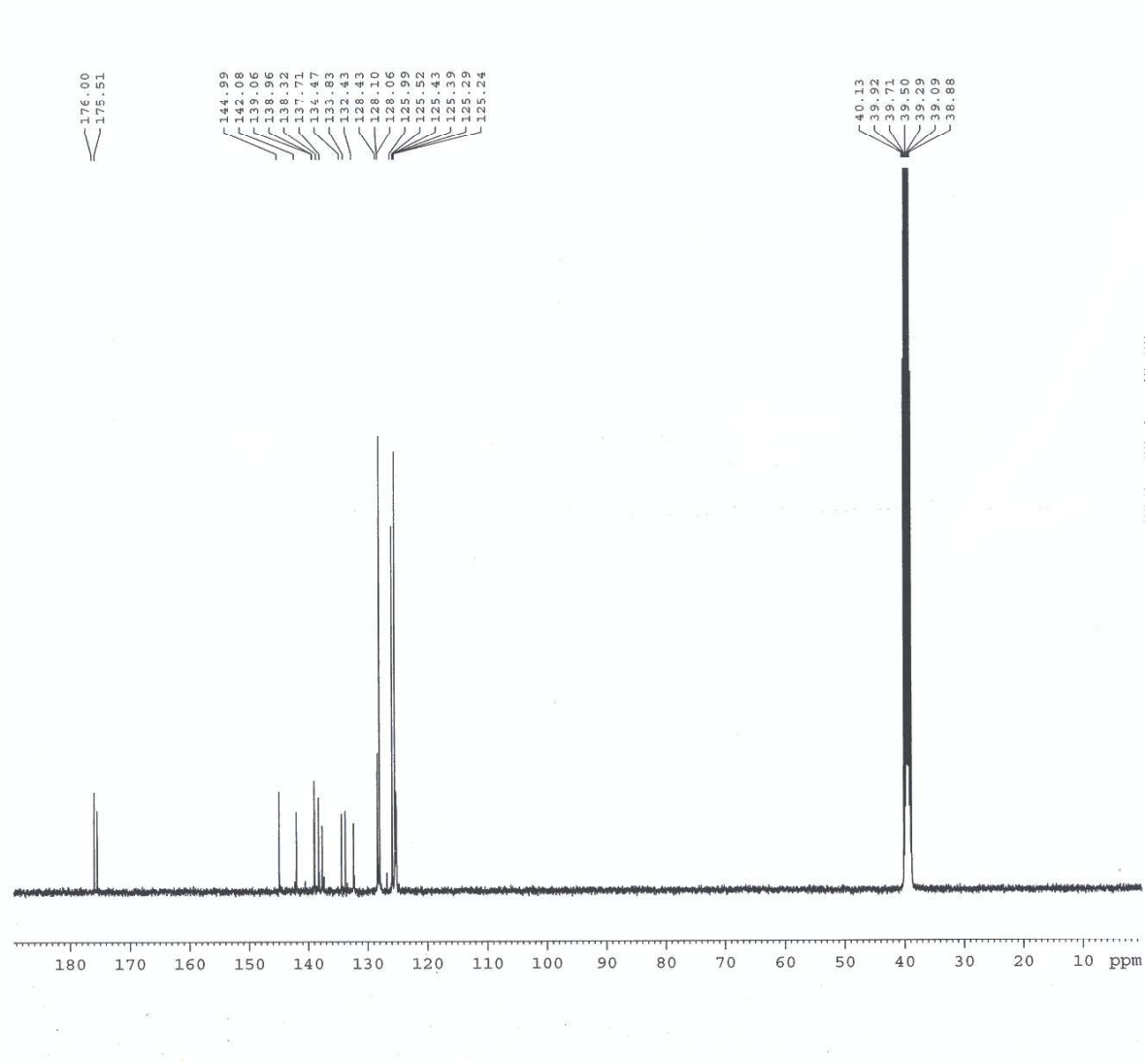
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144.99
142.08
139.06
138.96
138.32
137.71
134.47
133.83
132.43
128.43
128.10
128.06
125.99
125.52
125.43
125.39
125.29
125.24
40.13
39.92
39.71
39.50
39.29
39.09
38.88
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

Compound 1. Binding energy -3.612,0000 Kcal mol^{-1}

Center Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	C	-5,545	0,192	2,023
2	C	-4,362	-0,081	1,354
3	C	-4,347	-0,126	-0,052
4	C	-5,525	0,107	-0,767
5	C	-6,703	0,381	-0,078
6	C	-6,719	0,423	1,309
7	N	-3,087	-0,441	-0,673
8	C	-2,760	-0,385	-2,011
9	N	-1,388	-0,763	-2,288
10	N	-0,410	-0,333	-1,388
11	C	0,855	-0,440	-1,685
12	C	1,851	-0,044	-0,712
13	C	1,633	0,481	0,538
14	C	2,841	0,757	1,249
15	C	3,964	0,436	0,520
16	S	3,555	-0,214	-1,067
17	O	5,195	0,675	1,074
18	C	6,308	0,195	0,353
19	H	7,145	0,524	0,974
20	S	-3,721	-0,087	-3,329
21	H	-5,555	0,225	3,117
22	H	-3,450	-0,260	1,937
23	H	-5,514	0,083	-1,877
24	H	-7,622	0,563	-0,645
25	H	-7,651	0,638	1,843
26	H	-2,357	-0,583	-0,006
27	H	-1,159	-0,659	-3,259
28	H	1,225	-0,818	-2,654
29	H	0,646	0,674	0,965
30	H	2,854	1,177	2,257
31	H	6,303	-0,898	0,272
32	H	6,377	0,641	-0,646

Compound 1 deprotonated at H_f proton. Binding energy -3.616,6738 Kcal mol^{-1}

Center Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	C	-5,492	0,209	2,093
2	C	-4,271	0,049	1,447
3	C	-4,244	-0,138	0,057
4	C	-5,443	-0,152	-0,671
5	C	-6,647	0,013	-0,009
6	C	-6,679	0,190	1,373
7	N	-2,984	-0,372	-0,583
8	C	-2,753	-0,264	-1,991
9	N	-1,478	-0,124	-2,438
10	N	-0,472	0,058	-1,560
11	C	0,757	0,123	-2,017
12	C	1,842	0,329	-1,085
13	C	1,767	0,470	0,279
14	C	3,041	0,659	0,898
15	C	4,073	0,656	-0,008
16	S	3,497	0,423	-1,659
17	O	5,392	0,909	0,311
18	C	6,041	-0,186	0,925
19	H	7,038	0,211	1,135
20	S	-4,020	-0,411	-3,143
21	H	-5,514	0,351	3,178
22	H	-3,346	0,071	2,035
23	H	-5,302	-0,287	-1,828
24	H	-7,578	0,004	-0,583
25	H	-7,635	0,316	1,889
26	H	-2,220	-0,129	0,014
27	H	1,010	0,028	-3,084
28	H	0,834	0,443	0,845
29	H	3,162	0,786	1,975
30	H	5,549	-0,487	1,857
31	H	6,112	-1,050	0,256

Compound 1 deprotonated at H_g proton. Binding energy -3.609,6643 Kcal mol^{-1}

Center Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	C	-5,359	0,075	2,112
2	C	-4,208	-0,101	1,357
3	C	-4,281	-0,099	-0,048
4	C	-5,524	0,084	-0,672
5	C	-6,665	0,260	0,100
6	C	-6,590	0,256	1,488
7	N	-3,050	-0,289	-0,723
8	C	-2,859	-0,312	-2,023
9	N	-1,456	-0,582	-2,375
10	N	-0,436	-0,196	-1,593
11	C	0,804	-0,185	-2,031
12	C	1,869	0,160	-1,119
13	C	1,760	0,505	0,205
14	C	3,022	0,790	0,816
15	C	4,074	0,651	-0,055
16	S	3,536	0,167	-1,666
17	O	5,388	0,950	0,247
18	C	6,010	-0,015	1,069
19	H	7,003	0,411	1,232
20	S	-3,872	-0,159	-3,407
21	H	-5,299	0,073	3,204
22	H	-3,243	-0,242	1,857
23	H	-5,568	0,085	-1,783
24	H	-7,631	0,402	-0,393
25	H	-7,493	0,395	2,089
26	H	-1,304	-0,555	-3,368
27	H	1,088	-0,424	-3,069
28	H	0,813	0,562	0,745
29	H	3,118	1,079	1,863
30	H	5,489	-0,139	2,026
31	H	6,092	-0,987	0,572

Compound 2. Binding energy -3.785,9023 Kcal mol^{-1}

Center Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	C	-3,565	-0,573	1,346
2	C	-3,561	-0,757	-0,050
3	C	-4,748	-0,253	1,996
4	C	-5,932	-0,113	1,274
5	C	-5,926	-0,294	-0,103
6	C	-4,749	-0,617	-0,773
7	N	-2,300	-1,107	-0,649
8	C	-1,995	-1,219	-1,987
9	N	-0,610	-1,582	-2,237
10	N	0,358	-1,002	-1,436
11	C	1,633	-1,083	-1,765
12	S	-2,980	-1,130	-3,316
13	C	2,624	-0,527	-0,888
14	C	2,401	0,136	0,321
15	C	3,597	0,565	0,939
16	C	4,745	0,235	0,210
17	S	4,328	-0,621	-1,263
18	H	-2,645	-0,678	1,935
19	H	-4,750	-0,112	3,082
20	H	-6,863	0,140	1,793
21	H	-6,854	-0,184	-0,676
22	H	-4,749	-0,756	-1,875
23	H	-1,558	-1,148	0,018
24	H	-0,404	-1,630	-3,218
25	H	1,987	-1,559	-2,696
26	H	3,623	1,103	1,891
27	H	1,412	0,309	0,748
28	C	6,078	0,544	0,597
29	C	7,224	0,211	-0,127
30	C	8,421	0,650	0,504
31	C	8,181	1,308	1,690
32	S	6,503	1,407	2,065
33	H	7,209	-0,330	-1,076
34	H	9,412	0,477	0,082
35	H	8,944	1,730	2,343

Compound 2 deprotonated at H_f proton. Binding energy -3.792,1658 Kcal mol^{-1}

Center Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	C	-4,967	-2,256	-0,067
2	C	-4,173	-1,102	-0,158
3	C	-6,339	-2,132	0,117
4	C	-6,928	-0,876	0,216
5	C	-6,135	0,268	0,133
6	C	-4,768	0,168	-0,055
7	N	-2,775	-1,239	-0,406
8	C	-1,815	-0,2	-0,276
9	N	-0,614	-0,843	-0,215
10	N	0,519	-0,152	-0,188
11	C	1,667	-0,835	-0,121
12	S	-2,203	1,459	-0,266
13	C	2,894	-0,119	-0,095
14	C	3,075	1,27	-0,124
15	C	4,427	1,656	-0,089
16	C	5,319	0,571	-0,031
17	S	4,447	-0,951	-0,021
18	H	-4,523	-3,256	-0,139
19	H	-6,959	-3,031	0,185
20	H	-8,008	-0,788	0,36
21	H	-6,593	1,258	0,215
22	H	-4,017	1,06	-0,124
23	H	-2,443	-2,176	-0,298
24	H	1,708	-1,934	-0,086
25	H	4,756	2,697	-0,104
26	H	2,241	1,976	-0,17
27	C	6,731	0,678	0,011
28	C	7,626	-0,394	0,064
29	C	8,985	0,019	0,096
30	C	9,125	1,39	0,068
31	S	7,608	2,207	0,002
32	H	7,312	-1,439	0,078
33	H	9,817	-0,684	0,138
34	H	10,07	1,928	0,085

Compound 2 deprotonated at H_g proton. Binding energy -3.784,9167 Kcal mol^{-1}

Center Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	C	-4,736	-2,167	0,251
2	C	-4,100	-0,950	-0,060
3	C	-6,092	-2,186	0,543
4	C	-6,833	-1,008	0,532
5	C	-6,208	0,195	0,226
6	C	-4,852	0,235	-0,069
7	N	-2,718	-1,036	-0,344
8	C	-1,901	-0,048	-0,681
9	N	-0,630	-0,736	-0,965
10	N	0,534	-0,152	-0,654
11	C	1,670	-0,816	-0,659
12	S	-2,077	1,623	-0,887
13	C	2,896	-0,103	-0,401
14	C	3,051	1,242	-0,159
15	C	4,412	1,612	0,050
16	C	5,285	0,550	-0,033
17	S	4,433	-0,941	-0,374
18	H	-4,163	-3,101	0,262
19	H	-6,583	-3,134	0,784
20	H	-7,901	-1,031	0,763
21	H	-6,787	1,124	0,217
22	H	-4,337	1,188	-0,316
23	H	-0,648	-1,738	-0,886
24	H	1,746	-1,899	-0,852
25	H	4,717	2,641	0,255
26	H	2,224	1,956	-0,132
27	C	6,710	0,623	0,131
28	C	7,576	-0,446	0,126
29	C	8,941	-0,058	0,311
30	C	9,086	1,293	0,453
31	S	7,581	2,128	0,365
32	H	7,266	-1,484	-0,004
33	H	9,758	-0,778	0,334
34	H	10,026	1,818	0,605

Compound 3. Binding energy -4.174,4507 Kcal mol^{-1}

Center Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	C	-8,551	-0,153	0,042
2	C	-7,388	-0,552	0,695
3	C	-8,525	0,207	-1,299
4	C	-7,322	0,171	-2,002
5	C	-6,152	-0,222	-1,369
6	C	-6,180	-0,588	-0,009
7	N	-4,932	-1,005	0,571
8	C	-4,657	-1,290	1,891
9	N	-3,278	-1,683	2,123
10	S	-5,674	-1,375	3,195
11	N	-2,293	-0,999	1,428
12	C	-1,026	-1,134	1,763
13	C	-0,016	-0,464	0,991
14	C	-0,215	0,380	-0,101
15	C	0,999	0,878	-0,630
16	C	2,128	0,419	0,049
17	S	1,682	-0,644	1,363
18	C	3,479	0,783	-0,302
19	C	3,702	1,664	-1,377
20	C	4,997	2,026	-1,729
21	C	6,085	1,518	-1,019
22	C	5,873	0,644	0,048
23	C	4,582	0,276	0,409
24	H	-9,494	-0,126	0,600
25	H	-7,413	-0,834	1,768
26	H	-9,445	0,518	-1,805
27	H	-7,298	0,454	-3,060
28	H	-5,216	-0,242	-1,942
29	H	-4,172	-0,953	-0,076
30	H	-3,094	-1,854	3,094
31	H	-0,689	-1,740	2,622
32	H	-1,195	0,636	-0,507
33	H	1,071	1,559	-1,485
34	H	2,834	2,056	-1,929
35	H	5,162	2,712	-2,567
36	H	6,728	0,245	0,605
37	H	4,418	-0,411	1,249
38	H	7,104	1,805	-1,298

Compound 3 deprotonated at H_f proton. Binding energy -4.179,8892 Kcal mol^{-1}

Center Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	C	-8,838	0,378	-0,164
2	C	-7,471	0,280	0,022
3	C	-9,629	-0,767	-0,250
4	C	-9,039	-2,021	-0,156
5	C	-7,666	-2,145	0,026
6	C	-6,874	-0,989	0,121
7	N	-5,475	-1,126	0,369
8	C	-4,517	-0,085	0,238
9	N	-3,316	-0,724	0,172
10	S	-4,909	1,575	0,233
11	N	-2,183	-0,029	0,145
12	C	-1,035	-0,707	0,078
13	C	0,192	0,016	0,054
14	C	0,366	1,403	0,080
15	C	1,721	1,789	0,048
16	C	2,613	0,711	-0,002
17	S	1,749	-0,811	-0,013
18	C	4,043	0,859	-0,037
19	C	4,611	2,149	-0,024
20	C	5,991	2,311	-0,055
21	C	6,828	1,195	-0,099
22	C	6,276	-0,086	-0,112
23	C	4,897	-0,259	-0,082
24	H	-9,297	1,369	-0,242
25	H	-6,720	1,173	0,093
26	H	-10,710	-0,679	-0,392
27	H	-9,657	-2,922	-0,227
28	H	-7,220	-3,144	0,094
29	H	-5,142	-2,061	0,254
30	H	-0,987	-1,806	0,042
31	H	-0,469	2,107	0,121
32	H	2,069	2,827	0,062
33	H	3,937	3,018	0,011
34	H	6,422	3,317	-0,045
35	H	6,932	-0,962	-0,147
36	H	4,464	-1,267	-0,092
37	H	7,914	1,325	-0,122

Compound 3 deprotonated at H_g proton. Binding energy -4.172,6812 Kcal mol^{-1}

Center Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	C	-9,006	0,301	0,007
2	C	-7,618	0,346	-0,003
3	C	-9,679	-0,918	0,020
4	C	-8,951	-2,107	0,023
5	C	-7,563	-2,084	0,013
6	C	-6,878	-0,850	0,000
7	N	-5,472	-0,933	-0,010
8	C	-4,601	0,073	-0,027
9	N	-3,317	-0,626	-0,040
10	S	-4,746	1,759	-0,040
11	N	-2,149	-0,011	-0,021
12	C	-0,999	-0,707	-0,017
13	C	0,229	0,002	-0,008
14	C	0,408	1,391	-0,005
15	C	1,765	1,769	0,001
16	C	2,653	0,686	0,001
17	S	1,783	-0,834	-0,004
18	C	4,084	0,828	0,005
19	C	4,656	2,116	0,008
20	C	6,037	2,273	0,010
21	C	6,871	1,155	0,011
22	C	6,316	-0,125	0,008
23	C	4,935	-0,294	0,006
24	H	-9,575	1,236	0,004
25	H	-7,065	1,310	-0,014
26	H	-10,772	-0,944	0,027
27	H	-9,479	-3,066	0,033
28	H	-7,003	-3,025	0,016
29	H	-3,329	-1,630	-0,027
30	H	-0,964	-1,809	-0,019
31	H	-0,425	2,099	-0,007
32	H	2,118	2,805	0,004
33	H	3,984	2,988	0,007
34	H	6,471	3,278	0,012
35	H	6,970	-1,003	0,009
36	H	4,499	-1,301	0,003
37	H	7,958	1,281	0,013

Compound 4. Binding energy -4.547,5532 Kcal mol^{-1}

Center Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	C	-8,465	-0,002	0,023
2	C	-7,319	-0,428	-0,642
3	C	-8,417	0,352	1,366
4	C	-7,208	0,282	2,057
5	C	-6,055	-0,138	1,411
6	C	-6,105	-0,498	0,051
7	N	-4,873	-0,943	-0,543
8	C	-4,624	-1,250	-1,863
9	N	-3,256	-1,674	-2,109
10	S	-5,661	-1,331	-3,152
11	N	-2,247	-0,992	-1,444
12	C	-0,989	-1,161	-1,793
13	C	0,046	-0,492	-1,056
14	C	-0,118	0,395	0,007
15	C	1,114	0,881	0,504
16	C	2,224	0,370	-0,170
17	S	1,735	-0,727	-1,442
18	C	3,586	0,711	0,151
19	C	3,845	1,630	1,189
20	C	5,144	1,977	1,522
21	C	6,217	1,401	0,811
22	C	5,976	0,485	-0,225
23	C	4,667	0,147	-0,549
24	O	7,458	1,824	1,233
25	C	8,584	1,292	0,579
26	H	-9,412	0,052	-0,526
27	H	-7,362	-0,708	-1,716
28	H	-9,323	0,685	1,881
29	H	-7,167	0,560	3,115
30	H	-5,115	-0,184	1,976
31	H	-4,104	-0,899	0,093
32	H	-3,090	-1,865	-3,079
33	H	-0,678	-1,798	-2,640
34	H	-1,086	0,690	0,415
35	H	1,212	1,590	1,334
36	H	2,991	2,065	1,732
37	H	5,336	2,693	2,329
38	H	6,801	0,030	-0,786
39	H	4,474	-0,569	-1,358
40	H	9,409	1,784	1,101
41	H	8,659	0,204	0,699
42	H	8,607	1,548	-0,486

Compound 4 deprotonated at H_f proton. Binding energy -4.898,6172 Kcal mol^{-1}

Center Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	C	-8,805	0,395	-0,165
2	C	-7,437	0,310	0,020
3	C	-9,585	-0,758	-0,254
4	C	-8,981	-2,007	-0,162
5	C	-7,607	-2,116	0,020
6	C	-6,827	-0,952	0,116
7	N	-5,427	-1,074	0,364
8	C	-4,479	-0,023	0,234
9	N	-3,272	-0,649	0,168
10	S	-4,889	1,633	0,232
11	N	-2,146	0,057	0,141
12	C	-0,991	-0,609	0,078
13	C	0,229	0,126	0,054
14	C	0,389	1,515	0,073
15	C	1,740	1,914	0,046
16	C	2,643	0,845	0,007
17	S	1,794	-0,686	0,000
18	C	4,071	1,006	-0,019
19	C	4,628	2,302	-0,011
20	C	6,002	2,488	-0,029
21	C	6,850	1,363	-0,056
22	C	6,315	0,066	-0,067
23	C	4,935	-0,105	-0,048
24	O	8,197	1,676	-0,073
25	C	9,106	0,604	-0,069
26	H	-9,275	1,381	-0,241
27	H	-6,696	1,212	0,092
28	H	-10,666	-0,682	-0,396
29	H	-9,590	-2,913	-0,235
30	H	-7,151	-3,110	0,085
31	H	-5,084	-2,006	0,247
32	H	-0,933	-1,708	0,047
33	H	-0,453	2,211	0,106
34	H	2,078	2,956	0,055
35	H	3,943	3,164	0,012
36	H	6,423	3,499	-0,023
37	H	6,962	-0,817	-0,089
38	H	4,509	-1,116	-0,056
39	H	10,072	1,115	-0,070
40	H	9,013	-0,019	0,828
41	H	9,014	-0,024	-0,962

Compound 4 deprotonated at H_g proton. Binding energy -4.866,6987 Kcal mol^{-1}

Center Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	C	-8,856	0,316	0,313
2	C	-7,510	0,368	-0,021
3	C	-9,449	-0,884	0,690
4	C	-8,684	-2,046	0,732
5	C	-7,338	-2,015	0,400
6	C	-6,734	-0,802	0,018
7	N	-5,359	-0,875	-0,300
8	C	-4,571	0,113	-0,701
9	N	-3,295	-0,561	-0,996
10	S	-4,787	1,770	-0,970
11	N	-2,136	0,052	-0,707
12	C	-0,989	-0,591	-0,711
13	C	0,228	0,149	-0,480
14	C	0,361	1,499	-0,264
15	C	1,720	1,893	-0,077
16	C	2,610	0,847	-0,152
17	S	1,781	-0,663	-0,454
18	C	4,046	0,988	-0,002
19	C	4,593	2,258	0,236
20	C	5,960	2,428	0,380
21	C	6,804	1,310	0,286
22	C	6,275	0,038	0,051
23	C	4,901	-0,114	-0,091
24	O	8,147	1,605	0,446
25	C	9,055	0,538	0,346
26	H	-9,454	1,232	0,280
27	H	-7,020	1,318	-0,324
28	H	-10,510	-0,916	0,952
29	H	-9,150	-2,991	1,028
30	H	-6,747	-2,937	0,437
31	H	-3,294	-1,559	-0,877
32	H	-0,895	-1,676	-0,884
33	H	-0,476	2,201	-0,241
34	H	2,034	2,926	0,106
35	H	3,909	3,119	0,304
36	H	6,375	3,424	0,564
37	H	6,920	-0,844	-0,024
38	H	4,481	-1,111	-0,276
39	H	10,018	1,034	0,499
40	H	8,897	-0,219	1,123
41	H	9,033	0,061	-0,641

Compound 5. Binding energy -4.893,9375 Kcal mol^{-1}

Center Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	C	-8,423	-0,004	0,042
2	C	-7,283	-0,527	-0,561
3	C	-8,353	0,597	1,293
4	C	-7,128	0,681	1,952
5	C	-5,980	0,166	1,367
6	C	-6,053	-0,444	0,100
7	N	-4,826	-0,975	-0,430
8	C	-4,593	-1,498	-1,684
9	N	-3,227	-1,950	-1,878
10	S	-5,650	-1,797	-2,924
11	N	-2,213	-1,173	-1,337
12	C	-0,958	-1,399	-1,665
13	C	0,085	-0,626	-1,049
14	C	-0,070	0,418	-0,138
15	C	1,166	0,970	0,271
16	C	2,271	0,353	-0,318
17	S	1,770	-0,928	-1,400
18	C	3,635	0,732	-0,059
19	C	3,907	1,801	0,815
20	C	5,212	2,187	1,079
21	C	6,294	1,514	0,476
22	C	6,021	0,438	-0,392
23	C	4,714	0,055	-0,656
24	N	7,650	1,843	0,834
25	C	8,709	1,417	-0,109
26	C	7,888	3,213	1,343
27	H	-9,383	-0,071	-0,482
28	H	-7,343	-1,002	-1,563
29	H	-9,255	1,005	1,760
30	H	-7,069	1,154	2,938
31	H	-5,027	0,243	1,906
32	H	-4,047	-0,817	0,176
33	H	-3,072	-2,291	-2,808
34	H	-0,654	-2,162	-2,403
35	H	-1,035	0,778	0,223
36	H	1,272	1,800	0,979
37	H	3,062	2,324	1,287
38	H	5,401	3,022	1,771
39	H	6,850	-0,112	-0,862
40	H	4,518	-0,784	-1,336
41	H	9,668	1,408	0,425
42	H	8,510	0,398	-0,476
43	H	8,805	2,081	-0,981

44	H	8,842	3,224	1,886
45	H	7,935	3,970	0,545
46	H	7,090	3,506	2,045

Compound 5 deprotonated at H_f proton. Binding energy -4.898,6172 Kcal mol^{-1}

Center Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	C	-8,838	0,333	-0,105
2	C	-7,467	0,263	0,070
3	C	-9,603	-0,829	-0,206
4	C	-8,983	-2,071	-0,138
5	C	-7,606	-2,165	0,034
6	C	-6,841	-0,993	0,143
7	N	-5,437	-1,101	0,381
8	C	-4,504	-0,036	0,253
9	N	-3,290	-0,646	0,162
10	S	-4,934	1,614	0,282
11	N	-2,174	0,077	0,120
12	C	-1,010	-0,572	0,041
13	C	0,197	0,181	-0,006
14	C	0,334	1,573	0,003
15	C	1,678	1,995	-0,049
16	C	2,598	0,940	-0,098
17	S	1,775	-0,605	-0,082
18	C	4,021	1,126	-0,147
19	C	4,558	2,429	-0,155
20	C	5,929	2,635	-0,188
21	C	6,816	1,542	-0,211
22	C	6,282	0,239	-0,220
23	C	4,909	0,035	-0,187
24	N	8,244	1,753	-0,339
25	C	9,107	0,643	0,126
26	C	8,751	3,062	0,131
27	H	-9,320	1,313	-0,163
28	H	-6,737	1,172	0,151
29	H	-10,686	-0,764	-0,340
30	H	-9,580	-2,984	-0,221
31	H	-7,137	-3,154	0,081
32	H	-5,084	-2,027	0,245
33	H	-0,936	-1,670	0,012
34	H	-0,519	2,255	0,046
35	H	1,998	3,042	-0,052
36	H	3,861	3,282	-0,133
37	H	6,322	3,663	-0,202
38	H	6,956	-0,630	-0,258
39	H	4,506	-0,986	-0,192

40	H	10,109	0,775	-0,302
41	H	9,203	0,594	1,222
42	H	8,707	-0,322	-0,224
43	H	9,747	3,227	-0,300
44	H	8,088	3,873	-0,212
45	H	8,833	3,131	1,226

Compound 5 deprotonated at H_g proton. Binding energy -4.866,6987 Kcal mol^{-1}

Center Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	C	-8,702	0,502	-0,056
2	C	-7,339	0,254	-0,038
3	C	-9,6	-0,562	-0,049
4	C	-9,122	-1,873	-0,025
5	C	-7,762	-2,135	-0,008
6	C	-6,84	-1,064	-0,014
7	N	-5,479	-1,372	0,004
8	C	-4,524	-0,403	-0,013
9	N	-3,263	-0,935	-0,049
10	S	-4,847	1,33	-0,019
11	N	-2,152	-0,108	0
12	C	-0,933	-0,706	0,001
13	C	0,23	0,055	0,035
14	C	0,352	1,463	0,064
15	C	1,67	1,907	0,1
16	C	2,63	0,872	0,101
17	S	1,84	-0,693	0,053
18	C	4,038	1,095	0,137
19	C	4,544	2,413	0,168
20	C	5,908	2,656	0,194
21	C	6,826	1,587	0,185
22	C	6,328	0,27	0,171
23	C	4,962	0,028	0,145
24	N	8,252	1,837	0,307
25	C	9,137	0,758	-0,189
26	C	8,713	3,163	-0,165
27	H	-9,071	1,532	-0,075
28	H	-6,602	1,127	-0,041
29	H	-10,677	-0,371	-0,062
30	H	-9,834	-2,704	-0,02
31	H	-7,398	-3,168	0,01
32	H	-3,148	-1,925	-0,008
33	H	-0,829	-1,804	-0,022
34	H	-0,516	2,123	0,059
35	H	1,974	2,958	0,127
36	H	3,823	3,245	0,172

37	H	6,273	3,693	0,227
38	H	7,026	-0,58	0,186
39	H	4,587	-1,003	0,131
40	H	10,142	0,911	0,225
41	H	8,768	-0,222	0,154
42	H	9,217	0,726	-1,286
43	H	9,711	3,355	0,249
44	H	8,773	3,243	-1,261
45	H	8,033	3,951	0,196

Compound 6. Binding energy -4.370,7656 Kcal mol^{-1}

Center	**Atomic**	**Coordinates (Angstroms)**		
Number	**Type**	**X**	**Y**	**Z**
1	C	-8,498	-0,115	0,043
2	C	-7,339	-0,556	0,676
3	C	-8,471	0,297	-1,283
4	C	-7,270	0,273	-1,991
5	C	-6,104	-0,161	-1,377
6	C	-6,133	-0,579	-0,033
7	N	-4,889	-1,034	0,527
8	C	-4,617	-1,383	1,831
9	N	-3,238	-1,799	2,042
10	S	-5,630	-1,517	3,133
11	N	-2,249	-1,080	1,395
12	C	-0,984	-1,232	1,732
13	C	0,030	-0,521	1,004
14	C	-0,162	0,379	-0,044
15	C	1,054	0,907	-0,536
16	C	2,179	0,414	0,128
17	S	1,725	-0,716	1,380
18	C	3,530	0,801	-0,193
19	C	3,758	1,737	-1,220
20	C	5,051	2,126	-1,548
21	C	6,136	1,578	-0,848
22	C	5,925	0,644	0,176
23	C	4,629	0,259	0,501
24	C	7,462	1,973	-1,181
25	N	8,543	2,295	-1,453
26	H	-9,439	-0,098	0,604
27	H	-7,366	-0,881	1,737
28	H	-9,387	0,641	-1,773
29	H	-7,245	0,597	-3,037
30	H	-5,170	-0,171	-1,955
31	H	-4,130	-0,965	-0,119
32	H	-3,059	-2,031	3,002
33	H	-0,653	-1,884	2,560

34	H	-1,140	0,654	-0,444
35	H	1,130	1,632	-1,354
36	H	2,892	2,154	-1,756
37	H	5,219	2,856	-2,348
38	H	6,775	0,219	0,720
39	H	4,459	-0,471	1,302

Compound 6 deprotonated at H_f proton. Binding energy -4.379,4185 Kcal mol^{-1}

Center Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	C	-8,811	0,372	0,132
2	C	-7,439	0,274	-0,020
3	C	-9,603	-0,773	0,201
4	C	-9,009	-2,028	0,122
5	C	-7,633	-2,151	-0,027
6	C	-6,840	-0,994	-0,103
7	N	-5,434	-1,131	-0,312
8	C	-4,482	-0,089	-0,190
9	N	-3,276	-0,728	-0,128
10	S	-4,872	1,569	-0,185
11	N	-2,149	-0,031	-0,105
12	C	-0,994	-0,701	-0,046
13	C	0,224	0,033	-0,029
14	C	0,383	1,423	-0,053
15	C	1,733	1,822	-0,034
16	C	2,636	0,752	0,006
17	S	1,789	-0,777	0,023
18	C	4,062	0,915	0,026
19	C	4,617	2,212	0,009
20	C	5,992	2,396	0,024
21	C	6,840	1,279	0,056
22	C	6,305	-0,018	0,075
23	C	4,928	-0,196	0,060
24	C	8,250	1,462	0,070
25	N	9,402	1,611	0,081
26	H	-9,272	1,362	0,198
27	H	-6,690	1,168	-0,076
28	H	-10,686	-0,687	0,317
29	H	-9,628	-2,929	0,179
30	H	-7,184	-3,149	-0,084
31	H	-5,103	-2,067	-0,205
32	H	-0,939	-1,800	-0,013
33	H	-0,460	2,118	-0,086
34	H	2,070	2,864	-0,049
35	H	3,931	3,073	-0,017
36	H	6,412	3,407	0,010

37	H	6,970	-0,887	0,100
38	H	4,503	-1,208	0,073

Compound 6 deprotonated at H_g proton. Binding energy -4.372,0220 Kcal mol^{-1}

Center Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	C	-8,971	0,286	0,000
2	C	-7,584	0,332	0,000
3	C	-9,642	-0,932	0,000
4	C	-8,915	-2,119	0,001
5	C	-7,528	-2,094	0,001
6	C	-6,846	-0,862	0,000
7	N	-5,436	-0,944	0,000
8	C	-4,569	0,059	-0,001
9	N	-3,282	-0,643	-0,001
10	S	-4,698	1,746	-0,001
11	N	-2,114	-0,026	0,000
12	C	-0,969	-0,689	0,000
13	C	0,259	0,055	0,000
14	C	0,416	1,424	0,000
15	C	1,782	1,819	0,000
16	C	2,663	0,758	0,000
17	S	1,807	-0,767	0,000
18	C	4,103	0,902	0,000
19	C	4,668	2,186	0,000
20	C	6,044	2,354	0,000
21	C	6,876	1,229	0,000
22	C	6,326	-0,057	0,001
23	C	4,949	-0,216	0,000
24	C	8,289	1,395	0,000
25	N	9,442	1,530	0,000
26	H	-9,540	1,221	-0,001
27	H	-7,034	1,297	-0,001
28	H	-10,735	-0,959	0,000
29	H	-9,442	-3,078	0,001
30	H	-6,967	-3,035	0,001
31	H	-3,291	-1,648	0,000
32	H	-0,902	-1,788	0,000
33	H	-0,416	2,133	-0,001
34	H	2,115	2,862	-0,001
35	H	3,994	3,056	0,000
36	H	6,475	3,360	0,000
37	H	6,979	-0,936	0,001
38	H	4,512	-1,224	0,001